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**ANNUAL TECHNICAL REPORT
MATERIALS RESEARCH LABORATORY**
July 1, 1980-June 30, 1981



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Brown University
Providence, Rhode Island 02912

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ANNUAL TECHNICAL REPORT
MATERIALS RESEARCH LABORATORY

Brown University
Providence, RI 02912

A Report on Grant No. DMR-7923257

with the
National Science Foundation
Washington, DC 20550

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PREFACE

The Materials Research Laboratory at Brown University is engaged in interdisciplinary research directed toward the solution of problems in various areas of Materials Science.

In this report, Sections I-IV represent major thrust areas; the remaining sections are less extensive, since they cover either new areas of activity, emerging thrusts with a smaller number of investigators, or derive their principal funding from sources other than the NSF-MRL program.

Although the research summaries in this report are contributions from individual investigators, introductions to the four major thrust area summaries have been provided by investigators who during the reporting period assumed the functions of coordinators of those thrust areas. These are: Plasticity of Solids, R. J. Clifton; Fracture of Solids, L. B. Freund; Inorganic Glasses, W. M. Risen, Jr.; and Lower Dimensionality Materials and Structures, P. J. Stiles and C. Elbaum.

Since many of the research areas are interrelated, cross references have been made when the work might, with equal justice, have been placed in two or more sections.

The largest single source of support for this Laboratory is the Materials Science Branch of the National Science Foundation. Substantial support also came from thirteen other agencies and, of course, Brown University.

The Materials Research Laboratory at Brown University is administered by a Director, an Associate Director, and a committee composed of faculty members in representative areas of Materials Science.

The present appointees are:

Director:

G. S. Heller

Associate Director:

W. M. Risen, Jr.

Advisory Committee:

R. H. Cole
L. N. Cooper
P. J. Estrup
R. J. Clifton
J. Tauc

Those presently assuming the role of thrust area coordinators are:

Plasticity of Solids:

R. J. Clifton

Fracture of Solids:

L. B. Freund

Inorganic Glasses:

W. M. Risen, Jr.

Lower Dimensionality Materials and Structures:

P. J. Stiles

Solid Surfaces:

P. J. Estrup

Properties of Materials at Low Temperatures:

C. Elbaum

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SECTION 1

Plasticity of Solids

Introduction

Research in this thrust area is directed toward improving understanding of the plasticity of solids through relating macroscopic plastic response to underlying atomistic and microstructural scale mechanisms of plastic deformation. Materials studied include polycrystalline steel, aluminum, copper and α -titanium, as well as single crystal lithium fluoride and aluminum. Special attention is given to the effects of strain rate and temperature and to the mechanisms of strain localization. Strain localization investigations are reported under the Fracture of Solids thrust area because of their direct connection with ductile fracture.

Two primary experimental configurations used for investigating strain rate effects are the torsional Kolsky bar and the pressure-shear plate impact configuration. The former is advantageous for studying so-called strain rate history effects in which the strain rate is changed abruptly from 10^{-3} s^{-1} to 10^3 s^{-1} . The latter allows exceptionally high strain rates ($2 \times 10^5 \text{ s}^{-1}$) to be obtained. Interpretation of both types of experiments is relatively straightforward since the wave propagation is one-dimensional.

A series of strain rate change experiments on mild steel at room temperature and below indicated that the flow stress after an increase in strain rate is lower than the flow stress at the same strain when the straining occurs entirely at the higher strain rate (Duffy, Klepaczko). This stress difference is opposite to that observed previously for fcc and hcp metals. The stress difference decreases with increasing test temperature and becomes negligible at room temperature. Strain rate change experiments on LiF single crystals indicate that the flow stress increases sharply with increasing strain rate but that the effects of strain rate history are not pronounced (Duffy, Chiem). Modeling of dislocation mechanisms and microscopic observations of dislocation configurations are being used to gain insight into these phenomena.

Pressure-shear experiments on thin specimens of 1100-0 aluminum, 6061-T6 aluminum and OFHC copper indicate marked increases in flow stress at strain rates of 10^5 s^{-1} compared to reported values at 10^3 s^{-1} (Clifton, Li). For 1100-0 aluminum the large hydrostatic pressures (2-6 GPa) present in these experiments have been shown to have little influence on the increases in flow stress. Symmetric pressure-shear impact of plates of 6061-T6 aluminum and α -titanium have indicated that elementary elastic/visco-plastic models are inadequate for predicting the wave profiles that result (Clifton, Gilat). More attention needs to be given to modeling plastic response for complex stress paths in order to obtain agreement between predicted and observed profiles.

Dislocation dynamics in LiF single crystals have been investigated by means of elastic precursor decay and ultrasonic attenuation. Plate impact elastic precursor decay experiments designed to minimize the effects of surface damage indicate that precursor attenuation is reduced as surface damage is reduced (Clifton, Meir). Further improvement of surface quality is required before one can determine whether or not the larger than predicted precursor decay is due primarily to surface damage. Consideration of the elastodynamics of dislocation loops has been used to show that dislocation curvature does not affect precursor amplitudes at the wavefront (Clifton, Markenscoff). Attenuation of ultrasonic waves propagated at right angles to the axis of a crystal subjected to longitudinal stress pulses ($\sim 100 \mu \text{ sec}$ duration) has shown qualitative differences between the response of annealed and irradiated crystals (Elbaum, Hikata). Besides the expected differences in flow stress for the two conditions of the LiF crystals there are differences in the time histories of attenuation and velocity change during, and following, a stress pulse.

Dynamic plastic response of metal fiber, metal matrix composites has been investigated by means of transverse impact of beams (Kolsky, Mosquera). The main features of the response agree qualitatively with predictions of an elementary theory of fiber-reinforced rigid-plastic beams.

SECTION 1

Plasticity of Solids

Individual Contributions

Strain Rate and Strain Rate History Effects During Plastic Deformation

A torsional Kolsky bar has been employed to study the influence of strain rate as well as its history on the plastic flow stress of metals at dynamic rates. For this purpose a strain rate increment is imposed on tubular specimens during torsional deformation at a shear strain rate of $5 \times 10^{-4} \text{ s}^{-1}$. This increment raises the strain rate rapidly to 10^3 s^{-1} . In most metals, for instance in fcc and hcp metals, the imposition of the quasi-static prestrain results in a subsequent dynamic flow stress that is lower than that attained at the same total strain by straining entirely at the dynamic rate. For mild steel, however, it appears that the opposite is the case: the dynamic flow stress after a static prestrain overshoots that found by straining entirely at the dynamic rate. This effect is found to depend on temperature; it becomes progressively more pronounced as the test temperature is decreased. At room temperature no strain rate history effect is visible. An analysis of these results, in collaboration with Dr. J. Klepaczko and involving calculation of the thermal softening effect due to adiabatic heating during dynamic straining, indicates that this is not the only factor responsible for this history effect. It was concluded that another factor sharing responsibility for this behavior must involve structural changes that accompany plastic deformation such as a more intense rate of production of free dislocations in bcc metals at low temperatures. A model for yielding and plastic flow based on thermal activation and dislocation multiplication specific to BCC metals was derived. This model takes into account structural evolution and thus can account for strain rate history and temperature history effects. Numerical calculations performed for low carbon steels are compared with experimental data for 0.05% C annealed steel and AISI 1020 hot rolled steel. This comparison shows that the predictive possibilities of the model are quite good.

In addition, Dr. Klepaczko presented a discussion of a new experimental method for measuring fracture initiation toughness and high loading rates. To evaluate fracture initiation at a very high loading rate, he proposed using a special arrangement of the split Hopkinson pressure bar involving a wedge loaded specimen. Since the wedge is attached to the incident bar, the course of specimen loading and fracturing can be exactly monitored. This study was specifically devoted to estimating inertia and friction effects in the test.

A series of experiments was performed in which single crystals of LiF were loaded at various strain rates; following these tests microscopic observation was made of dislocation density and arrangement. The crystals were loaded quasi-statically and at high strain rates (10^3 s^{-1}) in shear. In addition, incremental strain rate experiments were performed in which a quasi-static prestrain was imposed before the dynamic loading. The results showed that the flow stress of LiF is strongly sensitive to strain rate but that the effects of strain rate history, although present are not pronounced. Microscopic observations using the etch pit technique showed that the dislocations are distributed uniformly after deformation at a constant quasi-static strain rate but that they congregate into wide bands as the result of incremental strain rate testing.

Principal Investigators: J. Duffy (Engineering) and J. Klepaczko (Engineering).

Personnel: R. H. Hawley (Engineering), G. J. LaBonte, Jr. (Engineering), P. Rush (Engineering), A. Rosakis (Engineering), A. Morrone (Engineering), K. Hartley (Engineering), Y. Zuiki (Engineering), E. Lavernia (Engineering), A. Asad (Engineering), P. Anderson (Engineering), and G. M. Meissner (Engineering).

Publications: "Strain Rate History Effects in LiF Single Crystals during Dynamic Loading in Shear," C. Y. Chiem and J. Duffy, *Material Science and Engineering* 48 (1981), 207-22.

"The Effect of Strain Rate and Strain Rate History on the Flow Stress of Aluminum Single Crystals," G. M. Meissner, R. H. Hawley, and J. Duffy, *Brown University Preliminary Report NSF CME79-23742/2*, December 1980.

"The Relation of Thermally Activated Flow in BCC Metals and Ferritic Steels to Strain Rate History and Temperature History Effects," J. Klepaczko, *MRL Technical Report, DMR-79-23257/2*, 1981.

"Strain Rate History Effects in Body-Centered Cubic Metals," J. Klepaczko and J. Duffy, presented at ASTM Symposium on Mechanical Testing, Bal Harbour, Florida, November 12-14, 1980; to be published in ASTM-STP on *Mechanical Testing for Deformation Model Development*.

"A Model for Yielding and Flow of Iron and BCC Metals Based on Thermal Activation," J. Klepaczko, DMR79-23257/132. NSF CME79-23742/4, June 1981.

Supported by the Materials Research Laboratory/NSF, the National Science Foundation, the Office of Naval Research, and the Army Research Office.

Plastic Shearing at Strain Rates of 10^5 s^{-1}

Thin specimens (0.2-0.4 mm thick) sandwiched between two high-impedance elastic plates have been subjected to strain rates of $6 \times 10^4 - 3 \times 10^5 \text{ s}^{-1}$ at pressures of 2 - 6 GPa by means of pressure-shear plate impact. Materials used for the specimens include 1100-0 aluminum, 6061-T6 aluminum, and OFHC copper. The elastic plates used as the flyer and anvil in the pressure-shear impact configuration have been made of either high strength steel or tungsten carbide. For all specimen materials there is a marked increase in flow stress over the values reported at strain rates of 10^3 s^{-1} and atmospheric pressure. Systematic variation of the velocity and angle of impact is being used to separate the effects of strain rate from the effects of hydrostatic pressure. For 1100-0 aluminum, which has been studied most thoroughly, it is evident that the large increase in flow stress is due almost entirely to the increase in strain rate.

Principal Investigator: R. J. Clifton (Engineering).

Personnel: C. H. Li (Engineering), R. M. Reed (Engineering), and L. Hermann (Engineering).

Publication: "Dynamic Stress-Strain Curves at Plastic Shear Strain Rates of 10^5 s^{-1} ," C. H. Li and R. J. Clifton, *Proceedings of the 1981 American Physical Society Topical Conference on Shock Waves in Condensed Matter* held at Stanford Research Institute, June 1981.

Supported by the United States Army Research Office, the Materials Research Laboratory/NSF, and the National Science Foundation.

Pressure-Shear Waves

Symmetric impact of parallel plates inclined relative to the direction of approach has been used to study the dynamic plastic response of 6061-T6 aluminum and α -titanium. Mathematical modeling of the experiments has been conducted using elastic-visco-plastic models for the response of the materials. Variations in the velocity and angle of impact are used to test the applicability of the models to a range of impact conditions. For α -titanium plates, comparison of computed and observed wave profiles suggests that neither an isotropic hardening model nor a kinematic hardening model is satisfactory. The computed stiffness of the material for shear in one direction after compression in another is overestimated by the isotropic hardening model and underestimated by the kinematic hardening model. Better agreement appears to be obtained for an independent hardening model in which plastic deformation causes hardening for subsequent loading along the same direction, but not for subsequent loading along orthogonal directions. For both materials the time profiles of transverse velocity are sufficiently sensitive to the visco-plasticity model used for the comparison of computed and observed profiles to allow many unsatisfactory models to be eliminated; however, limitations on the range of validity of acceptable models are not established readily.

Principal Investigator: R. J. Clifton (Engineering).

Personnel: A. Gilat (Engineering), L. Hermann (Engineering), and R. Reed (Engineering).

Supported by the National Science Foundation and the Materials Research Laboratory/NSF.

Dynamics of Dislocations in Single Crystals

A critical experiment is being developed for determining the effect of surface damage on the decay of the elastic precursor in plate impact experiments on single crystals. In this experiment the specimen is placed between two liquid layers to eliminate the damage due to impact of rough surfaces and to reduce the requirements on the flatness of the impact faces. With less stringent flatness requirements it appears possible to prepare surfaces which have adequate flatness and which have dislocation densities comparable to those in the bulk of the crystal. Preliminary experiments on LiF crystals shock-loaded through liquid layers of CH_2I_2 indicate that precursor amplitudes are increased as the surface damage is reduced. Whether or not the effect of surface damage is fully responsible for the smaller-than-predicted precursor amplitudes remains an open question. Further improvement in surface quality is required before the experiment can be regarded as a valid test of the plastic response of the bulk of the crystal. Such improvements appear possible.

Decay of the elastic precursor has been analyzed from the viewpoint of the elastodynamics of dislocations by considering elastic waves emitted from circular dislocation loops which begin to expand as the elastic precursor passes. This analysis yields the result that the rate of decay of the precursor depends on the initial dislocation configuration only through the mobile dislocation density, independent of the initial radii of the dislocation loops. It appears that better resolution of the near wavefront features may be necessary in both the analysis and the experiments before a definitive resolution of the precursor decay anomaly is obtained.

Principal Investigator: R. J. Clifton (Engineering).

Personnel: X. Markenscoff (Engineering) and G. Meir (Engineering).

Publications: "Elastic Precursor Decay and Radiation from Nonuniformly Moving Dislocations," R. J. Clifton and X. Markenscoff, J. Mech. Phys. Solids 29 (1981), 227.

"The Nonuniformly Moving Edge Dislocation," X. Markenscoff and R. J. Clifton, J. Mech. Phys. Solids 29 (1981), 253.

"Re-examination of the Precursor Decay Anomaly," R. J. Clifton, Proceedings of the American Physical Society 1981 Topical Conference on Shock Waves in Condensed Matter held at Stanford Research Institute.

Supported by the National Science Foundation and the Materials Research Laboratory/NSF.

Ultrasonic Studies of Dislocation Behavior Under Stress-Pulse Loading

We have previously described a system that we constructed for studying the dynamic behavior of dislocations during and immediately after the application of a short (~ 100 microseconds) duration stress pulse. This is accomplished by sampling at 10 microsecond intervals simultaneously the attenuation and velocity changes of a high frequency ultrasonic wave which propagates in the sample before, during and after the stress pulse. Preliminary experiments have been carried out on irradiated and on annealed lithium fluoride single crystals using this method. The results indicate, in addition to the expected differences in flow stress for the two types of crystals, a number of other distinctions. Most noteworthy are the following: 1) attenuation of [010] shear waves due to [100] longitudinal waves suggests that dislocation motion occurs on other than the primary slip systems $[110 \rightarrow 110]$; 2) the changes in ultrasonic attenuation and wave velocity do not reach their respective maxima at the same time; 3) the offset between the two maxima is different in annealed and in irradiated crystals; 4) following the passage of the stress pulse, recovery of attenuation and velocity during the first few hundred microseconds generally occurs at different rates; 5) in irradiated samples deformed elastically (below the yield stress), however, these recovery rates are not distinguishable; 6) in annealed samples for a given total change the differences in recovery rate are generally larger than in irradiated samples. These features are being analyzed in terms of dislocation dynamics.

Principal Investigator: C. Elbaum (Physics and Applied Mathematics).

Personnel: A. Hikata (Applied Mathematics) and S. F. Han (Physics).

Supported by the Materials Research Laboratory/NSF.

The Mechanical Response of Fiber Reinforced Materials

Work has been carried out on the elastic and plastic response of fiber reinforced solids. Two types of specimens have been employed in this work. The first is commercially available fiberglass epoxy composite; this type has been used primarily in studies of the dynamic elastic response of beams in flexure and in fracture studies. The other type of specimen was fabricated in the laboratory by embedding steel and phosphor bronze wires in matrices of lead and lead-tin alloys. The latter has been subjected to dynamic tests in a High-G testing machine; high speed cine-photographs and resistance strain gauge measurements were made simultaneously. More rapid testing by the detonation of explosive charges in contact with the specimens and by the impact of projectiles accelerated by such charges have also been carried out. It has been shown that at the highest rates of loading the response agrees, at least qualitatively, with the predictions of Spencer and his coworkers on the dynamic response of ideal fiber reinforced solids (1). This work has been the basis of a report (2) and a master's thesis (3), and has been presented as a paper to the 1981 annual meeting of the Society of Engineering Science.

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1. "Dynamics of Ideal Fiber-Reinforced Rigid-Plastic Beams," A. J. M. Spencer, J. Mech. Phys. Sol. 22 (1974), 147.
2. "Dynamic Loading of Fiber Reinforced Beams," J. M. Mosquera and H. Kolsky, 1981.
3. "Dynamic Loading of Fiber Reinforced Beams," J. M. Mosquera, Master's thesis, 1981.

Principal Investigator: H. Kolsky (Applied Mathematics).

Personnel: J. Mosquera (Engineering) and P. Russo (Applied Mathematics).

Publication: "The Dynamic Response of Fiber Reinforced Beams," H. Kolsky and J. M. Mosquera, paper read at the 18th annual meeting of S.E.S., Brown University, 1981.

Supported by the Materials Research Laboratory/NSF and the National Science Foundation.

Summaries of Other Related Work

Strength and Fracture of Two-Phase Alloys - J. Gurland (Engineering) - cf. Section 2.

Flow Localization in Porous Plastic Solids - A. Needleman (Engineering) - cf. Section 2.

Plastic Shear Localization from Inhomogeneous Deformation States - A. Needleman (Engineering) - cf. Section 2.

Single Crystal Plasticity - R. J. Asaro (Engineering) and A. Needleman (Engineering) - cf. Section 2.

Fatigue of Aluminum Alloys - R. J. Asaro (Engineering) - cf. Section 2.

Dynamic Elastic-Plastic Crack Growth - L. B. Freund (Engineering) - cf. Section 2.

Elastic-Plastic Stress Analysis of Cracks - J. R. Rice (Engineering) - cf. Section 2.

Fracture of Metals - J. Duffy (Engineering) - cf. Section 2.

Effects of Hydrogen on the Fracture of Steels - R. J. Asaro (Engineering) - cf. Section 2.

Ultrasonic Attenuation and Plastic Deformation in Solid Helium-Four - C. Elbaum (Applied Mathematics and Physics) - cf. Section 6.

SECTION 2

Fracture of Solids

Introduction

Research within the Fracture of Solids thrust area covers a wide range of experimental and theoretical topics concerned with the fracture of metals and alloys, as well as polymers and ceramics. A major objective of the work continues to be a comprehensive understanding of the relationship between material microstructure and phenomena on the microscale to macroscopic fracture behavior, as well as the characterization of the fracture resistance of materials. A total of ten faculty members from the Materials Science Group and the Mechanics of Solids Group, both within the Division of Engineering, and from the Division of Applied Mathematics contributed to work in this thrust area during the year. A number of graduate assistants, research associates, and support staff members were also involved. Summaries of work completed in the fracture area during the reporting period are presented in this section.

An area of major emphasis has been the influence of microstructure in fracture processes in metals. In research on fatigue crack growth in the age-hardenable aluminum alloys, the influence of grain size and precipitate type on initiation of fatigue cracks and on crack closure during cyclic loading has been clarified (Asaro, Hermann). Work on fracture initiation in steels under monotone loading has been carried out under both static and dynamic conditions in order to determine the mechanism of initiation, with particular attention on grain boundary carbide platelets in low carbon steels and on the role of prior austenite grain boundaries in eutectoid steels (Duffy, Hawley). Another project in this area has been concerned with ductile fracture in commercial dual phase steels with emphasis on roles of the individual phases (Gurland). The role of hydrogen in separation processes in carbon steels has also been studied (Asaro).

Work on the influence of microstructure has been paralleled by analyses of mechanical processes on the microscale in order to interpret data and to develop predictive capability. For example, the study of fatigue in aluminum included an analysis of crack closure and the results on closure have been interpreted in terms of models of crack tip plasticity. In work on the fracture toughness of cemented carbides, observations on the mechanisms of fracture have led to a model relating toughness with properties of the separate phases. Microscale models of the growth of cavities along grain boundaries in polycrystalline materials at high temperature have also been analyzed, with special attention on the relative importance of grain boundary diffusion and bulk creep in adjoining grains (Needleman, Rice).

Another area of emphasis has been the analysis of macroscopic crack growth in materials, including effects of nonlinear material response and inertia. The process of slow stable crack growth in ductile materials has been studied by means of detailed finite element models (Rice) and by means of simpler models amenable to exact analysis (Freund, Sills). In another numerical study of crack tip fields in ductile materials, the analysis was based on a corner theory of incremental plasticity and realistic localized plastic deformations were thereby induced in the blunted crack tip region (Needleman, Tvergaard). The area of dynamic crack growth in ductile materials has been particularly active, with emphasis on analyses to determine the influence of inertia on crack growth in elastic-plastic materials (Freund, Lo) and on the development of methods for measuring the dynamic fracture toughness of structural materials (Duffy, Freund).

Research on inhomogeneous plastic deformation as a precursor to ductile fracture has also been pursued jointly with the Plasticity of Solids thrust area. Attention has been directed toward understanding strain localization processes which might be encountered in the intensely deformed crack tip region in a ductile material due to reorientation of grains, yield locus vertex formation, or microvoid formation (Asaro, Needleman).

A variety of other projects have been carried out, including analysis and experiments on crack growth in brittle fiber reinforced composite materials (Kolsky, Pipkin), work on corrosive crack growth in reaction bonded silicon nitride (Richman), study of the wear properties of low stacking fault FCC materials (Avery), and consideration of criteria for design of structures against fracture which depart from traditional fracture mechanics (Broberg).

SECTION 2

Fracture of Solids

Individual Contributions

Fatigue of Aluminum Alloys

Research on fatigue of aluminum alloys has been concerned with a study of the macro- and micromechanics of fatigue crack growth in age-hardenable aluminum alloys, e.g., 2024 and 2048 aluminum. Special attention has been given to the influence of microstructure, in particular grain size and precipitate type, on the kinetics of crack growth and on such phenomena as crack closure. During the past year a detailed study of overload retardation has been carried out and the results have been successfully interpreted in terms of a simple closure model. More recent work has focused on fatigue crack initiation and again the influence of microstructure is of prime importance.

Our results have shown that crack tip closure is quite sensitive to grain size. In fact, we have shown that there is a transition in closure behavior in that the ratio K_{open}/K_{max} undergoes a rather abrupt fall from values near 0.5 to 0.2 at a K_{max} level consistent with the plastic zone size becoming comparable to the grain size. We have also found that closure levels are higher in underaged alloys which is consistent with our finding that crack growth rates are lowest in these microstructures. The results on closure have been interpreted in terms of models for crack tip plasticity and localized shearing. For plane strain crack growth closure results from the crushing of a rough fracture surface topology caused by the "zig-zag" sort to trajectory taken by the crack as it propagates along bands of concentrated shear.

This research has also led to the development and refinement of experimental techniques to measure very small increments of crack growth on the order of 0.005 mm. The program has also allowed us to build a computer interface to our closed loop testing machines which is now functioning as both a data acquisition system and as a controlling system.

Principal Investigator: R. J. Asaro (Engineering).

Personnel: L. Hermann (Engineering) and J-M. Baik (Engineering).

Publications: "Transitions in Fatigue Crack Closure in 2048 Aluminum," R. J. Asaro, L. Hermann, and J-M. Baik, *Met. Trans.* 12A (1981), 1133.

"Fatigue Crack Growth and Overload Retardation in 2048 Aluminum," J-M. Baik, L. Hermann, and R. J. Asaro, in *Mechanics of Fatigue*, ed. T. Mura, ASME Pub., AMD 47 (1981).

Supported by the Materials Research Laboratory/NSF and the AFOSR.

Fracture of Metals

We are continuing a study into the role of the microstructure during fracture initiation in structural steels under both static and dynamic conditions. It is now generally accepted that brittle fracture in very low carbon steels originates at carbide plates that form between ferrite grains. On the other hand, in eutectoid steels the fracture initiates in the pearlite and is governed by the prior austenite grain size. Most structural steels, however, have a carbon content which lies between these two limits, and preliminary results with an AISI 1020 hot-rolled steel seem to indicate that fracture can initiate either at the carbide plates or at the pearlite. This work involved both quasi-static and dynamic loading of notched round bar specimens and microstructural studies of the fracture surfaces. In order to study the role of the grain boundary carbide platelets, we have subjected specimens of 1020 steel to a heat treatment consisting of an isothermal transformation which reduces the size and number of the platelets, but has only a small effect on the yield point and the flow stress (the transformed steel shows a small increase in flow stress). In the fracture initiation tests this heat treatment resulted in a substantial increase in the fracture toughness, K_{Ic} , on the lower shelf where brittle fracture predominates. Using the optical and scanning electron microscopes, we traced the source of a number of the

microcracks located in or near the fracture surface in specimens of the transformed steel. It appears that some fractures originate at the carbide plates but others seem to initiate at the pearlite. In order to develop a clearer understanding of the fracture initiation process, it is important to pursue this investigation further. As a result, and in collaboration with Professor R. J. Asaro, we have embarked on a detailed investigation into the fracture initiation behavior of 1020 HRS specimens with controlled and predictable prior austenite and ferrite grain sizes. We shall now prepare fracture initiation specimens of 1020 HRS heat treated to vary the prior austenite and ferrite grain sizes as well as the size and number of carbide platelets. We should then be able to determine systematically the role of grain size and of carbide plates in the fracture initiation process. This will be accomplished by conducting static and dynamic fracture initiation experiments over a wide temperature range.

In conjunction with Professor L. B. Freund, we have started an investigation to attempt to relate the crack propagation behavior of metals to their fracture initiation properties. We have completed construction of a 12-frame Cranz-Schardin type camera system with an exposure time of one microsecond. It will be used to photograph caustic patterns produced at the crack tip during crack propagation. This method provides a direct measurement of the dynamic fracture toughness K_{I_d} at each station as well as crack propagation velocity. Immediate plans call for a series of experiments to determine fracture initiation toughness K_{I_c} and dynamic fracture toughness K_{I_d} for specimens of the same material.

In the crack propagation experiments we have made use of caustics to measure the values of K_{I_d} in a number of steels. However, we have found that the analysis of results made with this method needs to be extended to dynamic conditions and elastic-plastic behavior. The optical method of caustics has been used for some time by other investigators as a means for determining dynamic stress intensity factors in transparent materials. For these materials, the interpretation of the resulting shadow spots can be made using a static elastic crack model since most of these materials behave almost totally elastically up to fracture. Recently the method of caustics has been adapted to the measurement of stress intensity factors in metallic specimens by means of reflection from the metal surface also under the assumption of elastic deformation to fracture. In metals, however, plasticity and inertial effects must be considered. In a collaborative effort with Professor Freund, we have performed a shadow-spot analysis to determine the dynamic stress intensity factor of a rapidly running crack in the two-dimensional tensile mode using the Dugdale-Barenblatt line plastic zone model and performed experiments in which a crack propagates rapidly in a ductile steel. As a result one is now able to predict the shape of the caustic curve under conditions of plane stress and small scale yielding. The predicted and experimentally verified caustic curve under these conditions has geometrical features quite different from those found with purely elastic crack growth: it is considerably elongated in the crack direction. It was concluded that the error introduced through the neglect of plasticity effects can be large during crack propagation in common structural metals. More specifically, the criterion states that the error is large whenever the distance from the crack tip to the initial curve ahead of the tip is less than about twice the plastic zone size. (The initial curve is the locus of points on the specimen's surface which generate the caustic.) It was also determined that the error introduced through the neglect of inertial effects becomes significant when the crack speed is greater than about 20% of the longitudinal wave speed. The results showed that for materials in which the plastic zone size approached the initial curve or where crack speed is more than 20% of the longitudinal wave speed, the measured value of the stress intensity factor could be high by about 30-40% if plasticity and inertia are not properly taken into account.

Principal Investigator: J. Duffy (Engineering).

Personnel: R. H. Hawley (Engineering), G. J. LaBonte, Jr. (Engineering), P. Rush (Engineering), A. Rosakis (Engineering), Y. Zuiki (Engineering), E. Lavernia (Engineering), A. Asad (Engineering), and P. Anderson (Engineering).

Publications: "The Size and Density of Intergranular Carbide Plates in 1020 HRS and Their Role during Brittle Fracture Initiation: A Preliminary Report," J. C. Lambropoulos, R. J. Asaro, R. H. Hawley, and J. Duffy, Brown University Technical Report ARO DAAG29-80-K-0045/1, January 1981.

"The Effect of Crack Tip Plasticity on the Deformation of Dynamic Stress Intensity Factors by the Optical Method of Caustics," A. J. Rosakis and L. B. Freund, *J. Appl. Math.* 48 (1981), 302-08.

"Dynamic Fracture Initiation in Metals and Preliminary Results on the Method of Caustics for Crack Propagation Measurements," L. B. Freund, J. Duffy, and A. J. Rosakis, *Proceedings, Symposium on Analyses and Measurements of Dynamic Crack Propagation and Arrest, ASME Pressure Vessels and Piping Conference, Denver, 1981.*

"Discussion of a New Experimental Method in Measuring Fracture Toughness Initiation at High Loading Rates by Stress Waves," J. Klepaczko, Brown University Technical Report MRL E-131, May 1981.

Supported by the Materials Research Laboratory/NSF, the National Science Foundation, the Office of Naval Research, and the Army Research Office.

Strength and Fracture of Two-Phase Alloys

An analysis of the tensile deformation and fracture of a commercial dual-phase steel was conducted with emphasis on the roles that the individual phases have in these processes. It was observed that the deformation of ferrite is somewhat inhomogeneous, as suggested by the nonuniform appearance of slip lines in ferrite grains. The plastic deformation of martensite, as determined by changes in the particles' average aspect ratio, was found to be appreciable only at strains much higher than the uniform strain to necking. The mechanism of failure was one of void formation, growth, and coalescence. Void formation was observed to occur most frequently between the poles of two closely-spaced martensite particles situated on ferrite grain boundaries. Not surprisingly, then, martensite-induced void formation, growth, and coalescence initially occur in regions banded with martensite particles. Large inclusions were also observed to induce voids readily, and may contribute significantly to the fracture process. The applicability of theoretical models of void initiation, growth, and coalescence to the present steel, as well as some comparisons between the present two-phase steel and spheroidized steels, were also considered.

Principal Investigator: J. Gurland (Engineering).

Personnel: A. Scewczyk (Engineering) and H. Stanton (Engineering).

Publications: "An Investigation of the Tensile Deformation and Fracture of a Dual-Phase Steel," A. Scewczyk, Sc.M. thesis, July 1981.

"The Effect of Alloy Deformation on the Average Spacing Parameters of Non-Deforming Particles," J. Fisher and J. Gurland, *Metallurgical Transactions 12A* (1981), 167-71.

"Void Nucleation in Spheroidized Carbon Steels, Part I: Experimental Study," J. Fisher and J. Gurland, *Metal Science* 15 (1981), 185-92.

"Void Nucleation in Spheroidized Carbon Steels, Part II: A Comprehensive Model," J. Fisher and J. Gurland, *Metal Science* 15 (1981), 193-202.

Supported by the U.S. Department of Energy and the Materials Research Laboratory/NSF.

Effects of Hydrogen on the Fracture of Steels

Cialone and Asaro completed a study of the effect of hydrogen on the fracture of low to medium strength plain carbon steels. A preliminary report on their results appears in the July 1, 1980 Annual Technical Report. The work on plain carbon steels was extended to high strength steels, viz., 4140 steels tested in gaseous environments of pure dry hydrogen.

The results on two plain carbon steels, viz., a 1045 and a 1017 steel, along with those for a 0.15 wt. percent carbon steel showed that both the processes of void initiation and void growth are affected by hydrogen. Hydrogen was introduced electrolytically into the steels and specimens were deformed to various strains, up to and including complete fracture, and examined metallographically. Void initiation occurred at lower strain levels with hydrogen and the average void growth rate was increased by the presence of hydrogen. Void growth was found to be particularly accelerated along grain boundaries. Even when the fracture mode was unchanged then, this more rapid development of porosity caused reductions in ductility.

These observations of the effect of hydrogen on void initiation and void growth were interpreted in terms of a model for hydrogen induced losses in cohesion. The steels with the lower carbon contents (i.e., the 1017 and the 0.15 wt. percent C steels) displayed transitions in fracture mode. With increasing hydrogen contents the fracture mode shifted from the accelerated process of void initiation, growth and coalescence to one characterized by transgranular "quasi-cleavage." The latter mode was found to be very sensitive to the inclusion content and to the degree of coarseness of the microstructure. In fact, with regard to this latter point, a good correlation was found between the total amount of interface (grain boundary, particle-matrix, etc.) and the susceptibility to cleavage; the less total interface in the microstructure, the greater the tendency for cleavage.

The results on the high strength 4140 steels showed that hydrogen greatly affected fractures at inclusions, e.g., MnS particles. We were able to demonstrate that a critical stress criterion could be used to correlate the process of MnS steel matrix separation. We also found, however, that the fracture process beneath a sharp crack rarely involved inclusions but instead involved the fracture along martensite boundaries on prior austenite boundaries.

Principal Investigator: R. J. Asaro (Engineering).

Personnel: D. Groomes (Engineering).

Publication: "Hydrogen Assisted Fracture of Spheroidized Plain Carbon Steels," H. Cialone and R. J. Asaro, *Met. Trans.* 12A (1981), 1373.

Supported by the U.S. Department of Energy.

Plastic Shear Localization from Inhomogeneous Deformation States

In conjunction with V. Tvergaard of the Technical University of Denmark and M. Larsson and B. Storakers of the Royal Institute of Technology of Sweden, we have carried out a combined experimental and analytical study of instability and failure of internally pressurized ductile metal cylinders. Closed end cylinders made of an aluminum alloy and of pure copper and with several initial radius ratios were subject to internal pressure. The experiments show necking on one side of the tubes at a stage somewhat beyond the maximum internal pressure. The aluminum alloy tubes exhibited localized shear deformations in the neck region prior to fracture and all tubes, except for one of the aluminum alloy tubes, failed by shear fracture. A finite element analysis of the pressurized tubes was also carried out using the methods developed for analyzing shear localization problems developed in our previous study of plane strain tension (Tvergaard, Needleman, and Lo, *J. Mech. Phys. Solids* 29 [1981], 115). As in that study the material is characterized by the J_2 corner theory solid of Christoffersen and Hutchinson (*J. Mech. Phys. Solids* 27 [1979], 465). The theoretically predicted bifurcation into a necking mode, the cross sectional shape of the neck, and the initiation and growth of shear bands from the highly strained surface in the neck region were in good agreement with the experimental observations.

We have also, with V. Tvergaard, carried out an analysis of local crack tip stress and deformation fields for a solid characterized by the J_2 corner theory. Analyses of near tip fields, including the effects of the finite geometry changes which accompany crack tip blunting, play a role in relating continuum stress analyses to micromechanical failure mechanisms in the prediction of criteria for crack extension. They also provide a framework for assessing the degree to which a single parameter characterization of the crack tip fields is appropriate, since the blunted crack tip opening sets the size scale over which large strains and high triaxiality develop.

There are two immediate consequences of a vertex on the yield surface for crack tip fields; one is that near tip shear bands form due to the large local strains induced by blunting and the other is that the range of path independence of Rice's J integral is greater than indicated by an analysis based on classical smooth yield surface plasticity theory.

McMeeking and Parks (*ASTM STP668* [1979], 175) carried out an investigation of crack tip blunting using classical smooth yield surface plasticity theory and focused on the range of validity of a single parameter characterization of the near tip field. Our corresponding results, using J_2 corner theory, are in good agreement with theirs. However, the near tip fields given by the solid with a vertex on the yield surface differ substantially from those obtained using classical smooth yield surface plasticity theory in that intense shear bands develop. This is of significance since Green and Knott (*J. Engrn. Mat. and Tech.* 98 [1976], 37) and others have observed that toughness is reduced when the failure process involves localized shearing.

Our analysis gives an initial picture of shear band development at a crack tip. Further studies of shear band initiation and development and the relation to microstructural mechanisms of fracture are planned.

Principal Investigator: A. Needleman (Engineering).

Publications: "Flow Localization in the Plane Strain Tensile Test," V. Tvergaard, A. Needleman, and K. K. Lo, *Journal of the Mechanics and Physics of Solids* 29 (1981), 115-42.

"Instability and Failure Modes of Internally Pressurized Ductile Metal Cylinders," M. Larsson, A. Needleman, V. Tvergaard, and B. Storakers, submitted for publication.

"Crack Tip Stress and Deformation Fields in a Solid with a Vertex on its Yield Surface," A. Needleman and V. Tvergaard, submitted for publication.

Supported by the National Science Foundation and the U.S. Department of Energy.

Flow Localization in Porous Plastic Solids

Ductile metals, when highly deformed, are prone to the localization of deformation in the form of shear bands. Often such metals contain second phase particles which may crack or debond from the surrounding matrix material and the voids thus nucleated then grow by plastic deformation. A rate independent constitutive model of a porous plastic solid developed by Gurson has been employed to investigate the influence of void nucleation occurring during the deformation history on shear localization. Both plastic strain-controlled and stress-controlled nucleation processes are simulated. Two deformation histories are considered, one corresponding to uniaxial tension and the other to plane strain tension. The enhanced triaxiality at the center of a neck is simulated by application of Bridgman's solution for the stress and deformation state at the minimum section of a necked bar.

The plastic flow rule proposed by Gurson has been modified to account for material rate sensitivity. Comparisons are made with the results of a previous rate independent analysis (Saje, Pan, and Needleman, *Int. J. Fract.*, in press). Rate sensitivity is found to retard the onset of localization and the retardation is greater in plane strain tension than in axisymmetric tension. Also, in certain circumstances it is found that a stable excess shearing occurs in a rate sensitive solid, whereas a rate insensitive solid in these circumstances gives an unstable shear localization.

Principal Investigator: A. Needleman (Engineering).

Personnel: J. Pan (Engineering).

Publication: "Localization of Deformation in Rate Sensitive Porous Plastic Solids," J. Pan, M. Saje, and A. Needleman, submitted for publication.

Supported by the Materials Research Laboratory/NSF.

Rupture Processes at High Temperature

The growth of cavities along grain interfaces in polycrystalline materials at high temperature is a very complex problem. Under various conditions (e.g., different stress and temperature levels), the growth process can either be controlled by diffusion, by creep, or by the coupling of these two processes. Analytical expressions for the growth rates of the cavities can be obtained easily for the cases of grain boundary diffusion and dislocation creep in the adjoining grains when either process is the rate-controlled one.

The growth of cavities along grain interfaces by the combined processes under tensile loading conditions has been analyzed by Needleman and Rice. They have obtained numerical solutions by formulating a new variational principle and by implementing the principle through the finite element method. They have shown that the principal effect of the deformability of the adjoining grains is to shorten the diffusion path from the inter-cavity half-spacing to a distance of order L ahead of the cavity, with L being a stress and temperature dependent parameter of length dimension.

Sham and Needleman have extended the Needleman-Rice study to the investigation of the effects of triaxial stressing. These effects would be important, for example, in front of macro-cracks or notches where materials experience elevation in hydrostatic stress. The principal finding of the Sham-Needleman study is that the cavity growth rate for the coupled process under triaxial stressing conditions can be approximated by the sum of the individual contributions from the diffusion and creep process as if these two processes were acting alone, but properly account for the shortening of the diffusion path due to the deformability of the grains when the contribution to the cavity growth rate from the diffusion process is computed. The results of the Sham-Needleman study would provide a good model to analyze the growth of macro-cracks in polycrystalline materials by the mechanisms of growth and coalescence of micro-voids.

Principal Investigator: A. Needleman (Engineering).

Personnel: T-L. Sham (Engineering).

Supported by the U.S. Department of Energy.

Microstructure and Fracture Toughness of Cemented Carbides

The fracture processes of various WC-Co alloys were studied by observing 1) step by step surface crack growth on small double cantilever beam specimens using a specially constructed loading stage for the scanning electron microscope, 2) static internal cracks in epoxy-infiltrated specimens, and 3) matching fracture surfaces from single-edge-notch-beam specimens. The observed fracture process is WC-Co interface debonding and/or WC cracking by cleavage, followed by cobalt rupture. An attempt was made to describe the typical cobalt rupture modes.

Based on the observations of the cracking process, a model for the critical stress intensity factor, K_{IC} , has been proposed. In this model, the K_{IC} factor is based on the ductile tearing energy of the cobalt binder and is treated as a function of the microstructural parameters. Previously reported data fit fairly well to this model.

Principal Investigator: J. Gurland (Engineering).

Personnel: R. Deshmukh (Engineering), J. Hong (Engineering), and H. Stanton (Engineering).

Publications: "A Study of the Cracking Process and the Fracture Toughness of WC-Co Alloys," J. Hong, Ph.D. thesis, July 1981.

"Direct Observation of Surface Crack Initiation and Crack Growth in the Scanning Electron Microscope," J. Hong and J. Gurland, *Metallography* 14 (1981), 225-36.

Supported by the Materials Research Laboratory/NSF and the National Science Foundation.

Elastic-Plastic Stress Analysis of Cracks

Work has continued on the elastic-plastic analysis of cracks. The problems considered are: (1) quasi-static crack growth under rising load in rate-independent elastic-ideally plastic solids, and (2) step loading and time variable loading of cracked solids of rate-dependent creeping material.

In area (1), recent studies by Drugan, Rice, and Sham have completed a rigorous asymptotic analysis of the stress state at the tip of a growing crack under plane strain conditions. This differs from previous work in that no approximation is made which reduces the three-dimensional Mises yield condition to a two-dimensional, constant in-plane shear stress form. In the order in which they sweep over a point near the path of an advancing crack, the asymptotic field is found to be given by:

- (a) a plastic angular sector of constant Cartesian stress components,
- (b) a plastic "centered fan" sector in which singular plastic strains accumulate,
- (c) a non-singular plastic sector,
- (d) an elastic unloading sector, and
- (e) a further plastic loading sector bordering the crack surface.

Results for plastic strains and the like are given, and some progress has been made on the approximate determination of near tip parameters that are left unspecified by the asymptotic solution. This is done by comparison with a finite element simulation of stable crack growth by Sham.

In work on problem area (2), Kubo has extended his earlier studies on cracks in rigid-viscoplastic materials of the Bailey-Orowan type. The recent work includes consideration of transient effects due to elastic stress redistribution, and deals rigorously with step loading but less exactly with load variations such as unloading after a given hold time.

Principal Investigator: J. R. Rice (Engineering).

Personnel: S. Kubo (Engineering), W. J. Drugan (Engineering), and T-L. Sham (Engineering).

Publications: "Elastic-Plastic Crack Growth," J. R. Rice, in *Mechanics of Solids: The Rodney Hill 60th Anniversary Volume*, ed. H. G. Hopkins and M. J. Sewell, Pergamon Press, Oxford, 1981.

"Effects of Creep Recovery Hardening on the Stress and Strain Rate Fields near a Crack Tip in Creeping Materials," S. Kubo, in review for Proceedings 1981 ASTM Symposium on Elastic-Plastic Fracture, ASTM, Philadelphia.

"Combined Effects of Creep Recovery Hardening and Elastic Straining on the Stress and Strain Rate Fields near a Crack Tip in Creeping Materials," S. Kubo, submitted for publication.

Supported by the Materials Research Laboratory/NSF and the U.S. Department of Energy.

Analysis of Stable Crack Growth

Quasi-static growth of a crack in the antiplane shear mode through an elastic-plastic material has been analyzed. The material is taken to be nonhardening and small scale yielding conditions are assumed. The essential feature of the model is that the active plastic zone at the crack tip is comprised of a pair of discrete lines emanating from the crack tip, out of the plane of the crack, on which a suitable yield condition is enforced. For the case of steady growth, an exact solution is obtained for the plastic strain left in the wake of this active line plastic zone, and the extent of the plastic zone is determined in terms of the remote elastic stress intensity factor and the shear flow stress. The steady-state result is then coupled with a similar result for a stationary crack tip, and a particular ductile fracture criterion is adopted as a basis for considering some aspects of nonsteady growth. When the line of plastic yielding is perpendicular to the crack line, for example, it is found that the extent of the plastic zone from the tip is $0.071 (k/\tau_0)^2$ where k and τ_0 are the remote elastic stress intensity factor and the shear flow stress, respectively, and it is found that 36% of the elastic energy flowing into the crack-tip region during growth is dissipated through plastic work and 64% is trapped as residual elastic energy in the plastic-zone wake.

Principal Investigator: L. B. Freund (Engineering).

Personnel: L. B. Sills (Engineering).

Publications: "A Line Plastic-Zone Model for Steady Mode III Crack Growth in an Elastic-Plastic Material," L. B. Freund and L. B. Sills, *Journal of the Mechanics and Physics of Solids* 28 (1980), 49-57.

"The Line Plastic Zone Model for Growth of an Antiplane Shear Crack," L. B. Freund, in *Nonlinear and Dynamic Fracture Problems*, ed. W. Perrone and S. Atluri, AMD 35, ASME (1980), 171-83.

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Dynamic Elastic-Plastic Crack Growth

The study of the effects of inertia during steady-state antiplane shear crack growth in an elastic-ideally plastic material has been continued. First, an exact expression for the distribution of strain on the crack line within the primary active plastic zone has been obtained. It is shown that the expression reduces to the correct asymptotic form for the special case of vanishingly small distance from the crack tip for any nonzero crack growth speed, and it reduces to the correct limit as the crack speed approaches zero for any point on the crack line. Then, the full elastic-plastic deformation field has been determined under the conditions of small scale yielding by means of the numerical finite element method. The computed strain distribution on the crack line is found to compare closely with the analytic result for this distribution. Finally, the analytical and numerical results are combined with the "critical plastic strain at a characteristic distance" crack growth criterion to generate theoretical fracture toughness versus crack speed relationships. The results are similar to experimentally observed fracture toughness versus crack speed relationships. In particular, the results show a strong dependence of fracture toughness on crack speed for even moderate crack growth rates. Because the material response is independent of strain rate, this suggests that the influence of inertia on the fracture resistance of the material is significant.

Principal Investigator: L. B. Freund (Engineering).

Personnel: A. S. Douglas (Engineering).

Publications: "The Influence of Inertia on Elastic-Plastic Antiplane Shear Crack Growth," L. B. Freund and A. S. Douglas, Brown University Technical Report (1981), submitted for publication.

"Dynamic Fracture Toughness of Ductile Materials in Antiplane Shear," A. S. Douglas, Brown University Technical Report (1981); also Ph.D. thesis, Brown University.

Supported by the Materials Research Laboratory NSF and the National Science Foundation.

Dynamic Crack Propagation in Rate-Sensitive Materials

The asymptotic field of a propagating crack in an elastic-viscoplastic solid has been determined. The cases of anti-plane shear plane strain and plane stress were examined. The governing equations were reduced to a system of ordinary differential equations. This resulted in a two-point boundary value problem which was solved by a simple shooting scheme. Numerical results were obtained for anti-plane shear and plane strain. It was found that a minimum crack speed is required for stable propagation. The asymptotic result should also be useful for finite-element analysis of the same problem.

Principal Investigator: K. K. Lo (Engineering).

Personnel: C. Ma (Engineering).

Publication: "Dynamic Crack-Tip Fields in Rate-Sensitive Solids," K. K. Lo, submitted to JMPS, 1981.

Supported by the Materials Research Laboratory NSF.

Analysis of the Optical Method of Caustics in Fracture Mechanics

Work has been completed on analysis underlying the use of the optical method of caustics in dynamic fracture under small scale yielding conditions and in fully plastic quasi-static fracture. The shadow spot data which are obtained in using the method of caustics to determine experimentally dynamic stress intensity factors are usually interpreted on the basis of a static elastic crack model. In this work, an attempt was made to include both crack tip plasticity and inertial effects in the analysis underlying the use of the method of reflection. For dynamic crack propagation in the two-dimensional tensile mode which is accompanied by a Dugdale-Barenblatt line plastic zone, the predicted caustic curves and corresponding initial curves have been studied within the framework of plane stress and small scale yielding conditions. These curves have been found to have geometrical features which are quite different from those for purely elastic crack growth. Estimates have been made of the range of system parameters for which plasticity and inertial effects should be included in data analysis when using the method of caustics. For example, it is found that the error introduced through the neglect of plasticity effects in the analysis of data will be small as long as the size of the region near the crack tip which corresponds to the observed caustic is more than about twice the plastic zone size. Also, it is found that the error introduced through the neglect of inertial effects will be small as long as the crack speed is less than about 20% of the longitudinal wave speed. The analysis has been extended to include the effect of strain rate sensitivity on the plastic zone flow stress.

The possibility of measuring the plastic strain intensity factor deep within the crack tip plastic zone by means of the shadow spot method has also been studied. The value of the J-integral is adopted as the plastic strain intensity factor, and the lateral contraction of an elastic-ideally plastic planar specimen is calculated in terms of J from the nonhardening limit of the HRR asymptotic field of elastic-plastic fracture mechanics. The theoretical caustic curve which would be generated by geometrical reflection of normally incident parallel light from points of the deformed specimen surface lying well within the plastic zone is determined, and it is shown that the value of J is proportional to the maximum transverse diameter of the shadow spot to the third power. Results of preliminary experiments, in which values of J for a given single edge notched steel plate specimen are inferred from measurements performed separately from the elastically and plastically deforming parts of the specimen, have potential for use in ductile fracture testing.

Principal Investigator: L. B. Freund (Engineering).

Personnel: A. J. Rosakis (Engineering).

Publications: "The Effect of Crack Tip Plasticity on the Determination of Dynamic Stress Intensity Factors by the Optical Method of Caustics," A. J. Rosakis and L. B. Freund, *Journal of Applied Mechanics* 48 (1981), 302-08.

"Dynamic Fracture Initiation in Metals and Preliminary Results on the Method of Caustics for Crack Propagation Measurements," L. B. Freund, J. Duffy, and A. J. Rosakis, Paper No. 81-PVP-15, American Society of Mechanical Engineers (1981).

"Optical Measurement of the Plastic Strain Concentration at a Crack Tip in a Ductile Steel Plate," A. J. Rosakis and L. B. Freund, Brown University Technical Report (1981), submitted for publication.

Supported by the Materials Research Laboratory/NSF and the Office of Naval Research.

Single Crystal Plasticity

Pierce, Asaro, and Needleman are continuing work on large strain single crystal deformation. Constitutive relations were developed for the elastic-plastic deformation of single crystals which were specifically designed for use in finite element analyses. These relations precisely account for lattice rotations; the crystal hardening law is taken to be rate independent and both self hardening and latent hardening of the slip systems are accounted for. We have carried out finite element calculations, based on this constitutive law, of nonuniform and macroscopically localized deformation in single crystals deformed in tension. These calculations represent the first full solution to a boundary value problem involving a non-homogeneously deforming crystal. In the computations the crystal geometry is idealized in terms of the two-dimensional model introduced by Asaro. Essentially the model involves two possibly active slip systems which are in roughly primary-conjugate relation and are symmetrically oriented about the tensile axis before deformation begins.

The calculations follow the crystal through necking and the formation of shear bands and describe several important features of shear localization, in particular, which are in remarkably close agreement with experiments. For example, both the computed orientation of the material plane of the band and the computed lattice misorientations across the plane of the band are in close correspondence with those found experimentally. The calculations also uncovered some potentially important effects due to latent hardening. In the calculations when the latent hardening rates are sufficiently larger than the self hardening rates the deformation rapidly becomes "patchy." Observations of such "patchy" behavior in single crystals, as well as within grains of polycrystals, have been commonplace. Associated with this phenomenon of patchy slip are fundamental questions of uniqueness in the choice of active slip systems and in predicted lattice rotations. This has implications for the development of texture and for polycrystalline constitutive behavior.

Further theoretical studies of localization in single crystals and implications for polycrystalline behavior are planned.

Experimental studies of nonuniform and localized deformation in single crystals are being carried out by Lisiecki, Nelson, and Asaro. During the past year this work has focused on the development of patterns of nonuniform lattice orientation caused by necking and other nonuniform modes of plastic deformation. The materials used are pure single phase copper, alloys of copper-cobalt, and the aluminum-copper alloys previously studied by Chang and Asaro. The findings to date indicate that necking does indeed cause nonuniform lattice misorientations that lead to geometrical softening on some of the slip systems which in turn lead to localized shearing on those systems.

We have also found that the amount of necking that precedes localized shearing is largest in crystals characterized by lower strengths and higher strain hardening rates, as expected, and that the amount of lattice misorientation within the necks is also largest in the more deeply necking crystals. Shear bands in such deeply necking crystals tend to develop more gradually with strain as opposed to the rather abrupt formation process characteristic of strong, lower hardening crystals like aluminum-copper alloys. In the case of aluminum-copper crystals, Nelson has reconfirmed the earlier results of Chang and Asaro which showed that shear bands were geometrically softened by lattice rotations about the $\langle 110 \rangle$ direction that lies along the intersection between the primary and conjugate slip planes. This particular direction is that along which Lomer edge dislocations would lie and so we have suggested that the formation of tilt boundaries comprised of Lomer dislocations accounts for the observed misorientation and geometrical softening.

The theoretical findings discussed above are in very close agreement with these observations and together the experimental and theoretical studies have shown the importance of crystalline kinematics and related phenomena, such as the formation of local lattice misorientations, in causing shear band formation.

Principal Investigators: R. J. Asaro (Engineering) and A. Needleman (Engineering).

Personnel: D. Pierce (Engineering), L. Lisiecki (Engineering), and D. Nelson (Engineering).

Publications: "An Analysis of Nonuniform and Localized Deformation in Ductile Single Crystals," D. Pierce, R. J. Asaro, and A. Needleman, Brown University Report NSF/2 MRL/138, submitted to Acta Met.

"Micro and Macromechanics of Crystalline Plasticity," R. J. Asaro, Brown University Report NSF/3, to appear in Proceedings of the Workshop on Plasticity of Metals at Finite Strain, Stanford University, July 1981.

Supported by the Materials Research Laboratory/NSF.

The Fracture of Fiber-Reinforced Composites

The experimental and theoretical work on fracture propagation through samples of brittle fiber-reinforced solids has continued, and quasi-static and dynamic tests have been carried out on samples of brittle fiber-glass epoxy composites. Several novel phenomena have been observed. In particular it has been shown that for a fiber-glass epoxy composite (Scotchply 1002) which is reinforced by only a single family of parallel glass fibers, cracks propagate parallel to the fiber direction whatever the relative orientation of the applied tensile stress. For crossply specimens of the same material when rectangular specimens in which an edge notch has been cut parallel to one of the fiber directions are subjected to tensile loads perpendicular to the directions of the edge notch, the crack propagates in the direction perpendicular to the applied stress, i.e., in the direction of the notch, for some distance and then abruptly turns through 90° and progresses along the orthogonal fiber direction to an adjacent edge of the specimen. While this behavior is inexplicable in terms of conventional linear elastic fracture mechanics it has been shown by Professor Pipkin that the theory of ideal fiber-reinforced materials using a critical crack-tip force criterion predicts this type of behavior. The experimental observations have been shown to be in good qualitative agreement with the predictions of this theory. The work on the fracture strength of fiber-reinforced composites has been the basis of three papers, the first two of which are in press. Some experimental work on the dynamic response of these materials has also been commenced, but unlike the quasi-static tests in these studies on crossply specimens considerable amounts of delamination have been found to take place. The reasons for this are being studied.

Principal Investigator: H. Kolsky (Applied Mathematics).

Personnel: J. Mosquera (Engineering), G. Sun (Applied Mathematics), and P. Russo (Applied Mathematics).

Publications: "Fracture of Fiberglass Reinforced Composites," G. Sun, J. Composite Materials, 1981, in press.

"Crack Propagation in Unidirectional Fiber-Reinforced Materials," G. Sun, Engineering Fracture Mechanics, 1981, in press.

"An Experimental and Theoretical Study of Crack Propagation in Crossply Fiber Composites," G. Sun, H. Kolsky, and A. C. Pipkin, submitted for publication J. Engineering Mechanics, 1981.

Supported by the Materials Research Laboratory/NSF.

Failure of Fiber-Reinforced Materials

The theory of materials composed of inextensible fibers is so simple that it is feasible to predict the trajectories of dynamically advancing cracks, and to test proposed fracture criteria by comparing predicted and observed crack shapes. A doctoral thesis (1) and a paper based on it (2), setting up the basic theoretical framework for such problems, have been prepared. In a particular problem it is shown that under the maximum energy-release-rate criterion, the crack shape is circular, while under the so-called critical force and critical stress criteria, the crack runs parallel to one family of fibers, turns through a rounded corner whose size depends on the loading rate, and then runs out to the boundary parallel to the second family of fibers. Quasi-static experiments on Scotchply show the latter type of behavior.

A paper (3) has been prepared on dynamic propagation of a straight crack running parallel to one family of fibers. The problem is to determine the crack length as a function of time, for arbitrary histories of opening displacement at the edge of the sheet. The general method of solution was applied to two special problems. It was shown that in fast wedging, the crack speed oscillates above and below its limiting value, but approaches this limit very quickly. In slow wedging of an initially over-stressed crack, the crack propagates unstably at a constant speed, and crack arrest occurs when the strain has decreased sufficiently. The stress after arrest is well below the critical value for quasi-static propagation.

Two review articles on stress analysis (4) and fracture analysis (5) for fiber-reinforced materials were prepared.

Principal Investigator: A. C. Pipkin (Applied Mathematics).

Personnel: L. F. Mannion (Applied Mathematics).

Publications: (1) "Dynamic Fracture of Idealized Fiber-Reinforced Materials," L. F. Mannion, Ph.D. thesis, Brown University, 1981.

(2) "Dynamic Fracture of Idealized Fiber-Reinforced Materials," L. F. Mannion and A. C. Pipkin, in manuscript.

(3) "Crack Speeds in an Ideal Fiber-Reinforced Material," A. C. Pipkin, in manuscript.

(4) "Stress Channelling and Boundary Layers in Strongly Anisotropic Solids," A. C. Pipkin, CIME Lectures, Udine, 1981.

(5) "Fracture Mechanics of Fiber-Reinforced Materials," A. C. Pipkin, CIME Lectures, Udine, 1981.

Supported by the Materials Research Laboratory/NSF and the National Science Foundation.

Oxidation and Fracture Characteristics of Reaction Bonded Silicon Nitride (RBSN)

The application of high strength ceramic materials for high temperature components in gas turbine engines not only requires that these normally brittle materials have strength, toughness, and creep resistance at elevated temperatures, but also that they stand up to the hot corrosive and erosive atmospheres within the turbine engines. This requires that any oxidation of RBSN cannot result in the formation of surface flaws, oxide penetration of grain boundaries or internal oxidation of unreacted silicon in the volume of the material.

Experimental studies have been conducted on the oxidation of RBSN, the oxidation of nitrided single crystals of silicon and the development of reactive sputtered coatings, which resist oxidation at the surface and act as barriers to oxygen diffusion into the material. Surface pores act as sites for oxidation and can cause initiation of tensile cracks at the surface. These Griffith flaws can then propagate under the hydrostatic tensile stresses developed during thermal oxidation. Subsurface oxidation can also lead to similar consequences. If the subsurface porosity is connective, oxidation proceeds by kinetics similar to those for surface oxidation. If it is non-connective, solid state diffusion is required. In all cases, the oxide (cristobalite) formed at operating temperatures undergoes displacive transformation on cooling and a 5% volume increase occurs. This creates hydrostatic tensile stresses around the oxidation sites and brittle fracture can be initiated.

A method has been developed whereby reactively sputtered coatings of a hard, dense film of 3-5 μm of crystalline Si_3N_4 onto a porous RBSN surface results in substantial decrease in oxidation rates and prevents fracture under service conditions.

Principal Investigator: M. H. Richman (Engineering).

Personnel: O. J. Gregory (Engineering) and J. W. Fogarty (Engineering).

Publications: "Reactive Sputter-Coated RBSN," O. J. Gregory and M. H. Richman, to appear in J. Amer. Ceram. Soc.

"Nitridation of High Purity-Single Crystal Silicon," O. J. Gregory and M. H. Richman, to appear in Metallography.

"Strength and Fracture Toughness of Reaction Bonded Si_3N_4 ," S. C. Danforth and M. H. Richman, to appear in J. Amer. Ceram. Soc.

Supported by the Materials Research Laboratory/NSF and NASA/Lewis.

Shear Localization and Fracture in Abrasive Wear

Resistance of materials to abrasive wear has great economic and strategic importance, particularly in the areas of mining, minerals processing and plastic processing. Traditionally, materials have been selected on the basis of hardness. Certain classes of alloys, however, comprising low stacking fault f.c.c. materials, notably aluminum bronzes, stainless steels, Ni-Cr-B (chromalloys) and particularly Co-Cr-W (Stellites), have shown far greater wear resistance than comparable iron-based alloys of similar hardness. Current theory ascribes a strong role to shear localization and fracture in abrasive wear.

Titanium-cobalt alloys show considerable promise as cobalt-chromium substitutes. Stacking fault energy is very low and the alloys are extremely resistant to shear localization. Our previous work has centered on thermomechanical processing of these alloys to develop ultra high strength. The deformation-aging cycle (40-90% cold work followed by low temperature aging 150-400°C) is very close to the surface deformation conditions encountered in abrasive wear. Thus the surface should transform to a condition of maximum strength under wear conditions.

Test samples of five different titanium-cobalt alloys have been prepared by vacuum melting to form 500 gram ingots. These were hot forged, machined, and cold rolled to strip. They are now being subjected to abrasive wear testing in the annealed, cold rolled, and thermomechanically aged state. Metallographic sectioning will be used to look for shear delamination below the wear surface.

Principal Investigator: D. H. Avery (Engineering).

Supported by the Materials Research Laboratory/NSF.

The Foundation of Fracture Mechanics

Our research has concerned the foundations of currently practiced fracture mechanics and the possibility of establishing a fracture mechanics that could be used in engineering. In addition we have solved a mathematical problem about crack propagation in a layer.

Fracture mechanics of monotone loading is, in our opinion, a poorly developed discipline with a very limited practical applicability. The theoretical and experimental foundations were investigated. Neither seems to permit extension beyond the linear fracture mechanics. We also investigated the sensitivity of structures to repeated loading and found that situations can exist in which only a few tens of major load applications give significantly lower strength than the one at one load application.

We have made a detailed suggestion of a fracture mechanics intended for a moderately low number of load cycles. The suggestion involves more simple routines than currently practiced fracture mechanics of monotone loading in the non-linear range.

A somewhat different problem concerned fast crack propagation in a layer. In previous investigations crack tip velocities that are subsonic with respect to the surrounding medium and either subsonic or supersonic with respect to the layer have been studied. Here the crack tip velocity was assumed to be supersonic with respect to the surrounding medium and subsonic with respect to the layer.

Principal Investigator: K. B. Broberg (Engineering).

Publications: "The Foundations of Fracture Mechanics," submitted to the Engineering Fracture Mechanics.

"Toward a New Fracture Mechanics," submitted to the Journal of Engineering Mechanics and Technology.

"Crack Propagation in a Layer," submitted to the International Journal of Fracture.

Supported by the Materials Research Laboratory/NSF.

Summary of Other Related Work

Strain Rate and Strain Rate History Effects during Plastic Deformation - J. Duffy (Engineering) and J. Klepaczko (Engineering) -
cf. Section 1.

SECTION 3

Inorganic Glasses

Introduction

The Inorganic Glasses Group focuses its research on understanding the structures, relaxation phenomena, and electronic states and properties of the three main types of inorganic glasses; oxide glasses, amorphous semiconductors, and amorphous metals. Fundamental issues concerning the amorphous state are being addressed by studying each of these types of materials and by developing new theoretical and experimental methods for their investigation.

The first direct observation of ultrafast processes of thermalization of hot carriers in amorphous semiconductors, whose existence was implied indirectly from previous steady state studies of photoconductivity, is reported. From these first experimental data on the actual rates, it was possible to identify the kind of electron-phonon interaction that dominates the process. In addition, based on new time-resolved spectroscopic studies on photoinduced midgap absorption in amorphous tetrahedrally bonded semiconductors, support was developed for Tauc's proposal that electron-transport dominates the recombination process while the induced absorption itself is due to the photoinduced transition of trapped holes into the valence band.

The previous report from this Group that ultrasonic attenuation as a function of amplitude frequency and temperature in certain metallic glasses does not behave in accordance with two-level-system tunneling theory has led to newly reported work carried out over a wide range of frequencies and with additional metallic glass compositions. It is shown that the effect is not continued to the frequency, temperature, or compositions first studied. The frequency and temperature dependence of the completely saturated attenuation is reported.

Theoretical studies reported include the calculation of the effects on resistance and Hall resistance of two-dimensional disordered electronic systems due to interactions in the strong field limit, where localization effects are suppressed. And, continued experimental work on time-domain spectroscopy has led to development of new and more powerful methods for measuring very small dielectric losses in the 500 KHz to 250 MHz range (potential limit 2 GHz) with 10 psec resolution and 1 psec reproducibility.

The structures of inorganic oxide glasses have been the subject of a number of new studies. In a Raman study of the polarization dependence of molecular orientation in B_2O_3 films, evidence for the existence and preferential orientation of the boroxyl group was obtained. The existence of this grouping also was employed to interpret the structural effects of thermal treatment on $MgO \cdot B_2O_3$ materials studied by NMR. A theoretical model for high temperature defects in fused silica, based on bond breaking and reformation processes, has led to a new peroxy bridge model to interpret anomalous Raman observations. The reported structural studies of ionic oxide glasses by NMR, laser Raman and far infrared spectra include data and interpretations on fast ionic conduction and mechanical relaxation. Structural changes which occur as composition and preparation methods are varied also are reported.

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SECTION 3

Inorganic Glasses

Individual Contributions

Time Resolved Spectroscopy of Photoinduced Midgap Absorption

We continued our studies of the photoinduced midgap absorption band in amorphous tetrahedrally bonded semiconductors in two directions: time evolution of the total band strength and of its spectrum. The studied material was amorphous hydrogenated silicon. The time domain was 500 nsec to 100 msec, the spectral range was 0.7 to 1.3 eV, the temperature range from 10 to 300K.

We showed that from the decay of the total band strength with time one can learn about the dynamics of electrons. We presented evidence that the recombination rate depends on the intensity of illumination and argued that the recombination is bimolecular. We showed that in amorphous hydrogenated Si prepared by the glow discharge method the electron transport can be described by a multiple trapping model with an exponential distribution of electron traps in the gap while in the material prepared by sputtering tunneling effects often appear to be important. The dispersion constants that describe the transport of electrons in these materials obtained from our data are in reasonable agreement with the values obtained from the flight-of-time method for electrons. This supports our proposal that the electron transport dominates the recombination process while the induced absorption itself is due to the photoinduced transition of trapped holes into the valence band.

The data on the time evolution and temperature dependence of the spectra give us information about the energy distribution of hole traps and the change of their occupation with time. In glow-discharge material an exponential trap density distribution explains the data remarkably well, indicating that the multiple trapping model is applicable for holes. The data on sputtered materials were not so easy to interpret; the trap distributions appear to be non-exponential and the theory is more complex.

Principal Investigator: J. Tauc (Engineering and Physics).

Personnel: Z. Vardeny (Engineering) and P. O'Connor (Physics).

Publications: "Photoinduced Midgap Absorption in Tetrahedrally-Bonded Amorphous Semiconductors," P. O'Connor and J. Tauc, to appear in Phys. Rev.

"Recombination Kinetics in a-Si:H," Z. Vardeny, P. O'Connor, S. Ray, and J. Tauc, Phys. Rev. Lett. **46** (1981), 1108.

"Relaxation of Photoinduced Sub-Bandgap Absorption in a-Si:H," S. Ray, Z. Vardeny, J. Tauc, T. Moustakas, and B. Abeles, AIP Conference Proceedings **73**, 253.

"Time Resolved Spectroscopy of Photoinduced Absorption in Glow-Discharge a-Si:H," S. Ray, Z. Vardeny, and J. Tauc, Proc. 9th Intl. Conf. Amorphous and Liquid Semiconductors, Grenoble (1981).

Supported by the Materials Research Laboratory/NSF and the National Science Foundation.

Thermalization of Hot Carriers in Amorphous Semiconductors

We improved the stability and the signal-to-noise ratio of our subpicosecond pump and probe experimental set-up and were able to study electronic relaxation effects from 0.5 psec to 10 psec with a 0.1 psec resolution. Below 2 psec the main problem was the so-called "coherent artifact" produced by the interaction of the coherent fields of the pump and probe pulses during their overlap. We developed a deeper understanding of the origin of this effect and showed that under certain conditions, usually satisfied in amorphous semiconductors, the artifact can be removed by using perpendicular polarizations of the pump and probe beams. This opened up for us the possibility to study the thermalization processes of photogenerated hot carriers. We studied them in

amorphous Si, hydrogenated and fluorinated Si and glassy As_2Se_3 and Se. We measured the rates of the dissipation of the hot carrier excess energy (e.g., 0.5 eV psec in a-Si, 0.1 eV psec in a-Si:H) and showed that the dissipation occurs via interaction with polar phonons (Frohlich interaction) with the exception of a-Si in which it is considerably higher; in this latter case the electron-phonon interaction is apparently enhanced at the defects present in large concentrations in this material. This work is the first direct observation of the ultrafast thermalization processes whose existence was indirectly implied from previously steady state studies of photoconductivity and other effects and our results agree in the broad features with conclusions of the previous work. However, we obtained first experimental data on the actual rates and were able to identify the kind of the electron-phonon interaction that dominates the process.

Principal Investigator: J. Tauc (Engineering and Physics).

Personnel: Z. Vardeny (Engineering) and J. Strait (Physics).

Publications: "Hot Carrier Thermalization in Amorphous Silicon," Z. Vardeny and J. Tauc, Phys. Rev. Lett. 46 (1981), 1227.

"Optical Picosecond Studies of Carrier Thermalization in Amorphous Silicon," Z. Vardeny, J. Tauc, and C. J. Fang, AIP Conference Proceedings 73, 243.

"Picosecond Coherence Coupling in the Pump and Probe Technique," Z. Vardeny and J. Tauc, to appear in Optics Communications.

"Picosecond Dynamics of Carriers in Amorphous Semiconductors," Z. Vardeny, J. Tauc, and C. J. Fang, Proc. 9th Intl. Conf. Amorphous and Liquid Semiconductors, Grenoble (1981).

"Picosecond Dynamics of Carriers in Amorphous Semiconductors," J. Tauc, submitted to Revue Roumaine de Physique.

"Optical Picosecond Studies of Hot Carriers in Amorphous Semiconductors," Z. Vardeny and J. Tauc, Proc. 3rd Intl. Conf. on Hot Carriers in Semiconductors, Montpellier (1981).

Supported by the Materials Research Laboratory/NSF and the National Science Foundation.

Instantons and Disordered Systems

We have continued our work on disordered systems. We calculate the corrections to the resistance R and Hall resistance R_H of a two-dimensional disordered electronic system due to interactions in the strong field limit $\omega_c \tau \gg 1$ where localization effects are suppressed. We find that $\Delta\sigma_{xy} = 0$ for both $\omega_c \tau \gg 1$. With the result that $(\delta R_H/R_H)/(\delta R/R) = 2/(1 - (\omega_c \tau)^2)$ oscillating with field because of the field dependence of τ and eventually diverging when $(\omega_c \tau) = 1$. $\delta R/R$ decreases with increasing field going through zero when $\omega_c \tau = 1$. It has also been shown that there are similar logarithmic corrections to the heat current in two dimensions from both localization and interaction effects. Measurement of the thermoelectric power is a convenient way of separating the two phenomena.

Principal Investigator: A. Houghton (Physics).

Personnel: J. R. Senna (Physics) and H. J. Kim (Physics).

Publications: "Correction to Scaling Amplitude Ratios for the Superfluid Transition in ^4He ," A. Houghton and M. C. Chang, Phys. Rev. B 23 (1981), 1473.

"Noncompact σ Models and the Existence of a Mobility Edge in Disordered Electronic Systems near Two Dimensions," A. Houghton, A. Jevicki, R. D. Kenway, and A. M. M. Pruisken, Proceedings of the Intl. Conf. on Statistical Mechanics, Edmonton, Alberta, Canada, 1980.

"Magnetoresistance and Hall Effect of a Disordered Interaction Two-Dimensional Electron Gas," A. Houghton, J. R. Senna, and S.-C. Ying, J. Non-Cryst. Solids, to be published.

"Thermoelectric Power in Two-Dimensional Disordered Systems," A. Houghton, J. R. Senna, and C. S. Ting, J. Non-Crystl Solids, to be published.

"Magnetoresistance and Hall Effect of a Disordered Interacting Two-Dimensional Electron Gas," A. Houghton, J. R. Senna, and S-C. Ying, Phys. Rev. B, to be published.

"Magnetoeconductance of a Disordered Interacting 2-D Electron Gas," A. Houghton, J. R. Senna, and S-C. Ying, Physica, to be published.

"Thermoelectric Properties of Two-Dimensional Systems," A. Houghton, J. R. Senna, and C. S. Ting, Phys. Rev. B, to be published.

Supported by the Materials Research Laboratory NSF and the National Science Foundation.

Ultrasonic Studies of Metallic Glasses

We have previously reported the observation that in the metallic glasses $\text{Pd}_{0.775}\text{Si}_{0.165}\text{Cu}_{0.06}$ at low temperatures (below 1K) ultrasonic attenuation as a function of amplitude, frequency and temperature does not behave in accordance with predictions of the two-level-system (TLS) tunneling theory. The observations were based on experiments in the frequency range 10-90 MHz. In order to establish whether these results were confined to low frequencies and to the above-mentioned composition, a study was carried out on metallic glasses of different compositions ($\text{Pd}_{0.80}\text{Si}_{0.20}$ and $\text{Pd}_{0.40}\text{Ni}_{0.40}\text{Si}_{0.20}$) in the frequency range 10-700 MHz. Contrary to the predictions of the TLS theory, a linear frequency dependence and essentially no temperature dependence of the total saturable attenuation changes were found for both alloys. These results extend the previous ones on $\text{Pd}_{0.775}\text{Si}_{0.165}\text{Cu}_{0.06}$. In addition, the frequency and temperature dependence of the completely saturated attenuation is found to have the form $\omega^{-n}(T/T_0)$ at temperatures 0.3-2K.

Principal Investigator: C. Elbaum (Physics and Applied Mathematics).

Personnel: A. Hikata (Applied Mathematics) and G. Park (Physics).

Publications: "Ultrasonic Studies of the Amorphous Binary Alloy $\text{Pd}_{0.82}\text{Si}_{0.18}$ at Low Temperatures," G. Park, A. Hikata, and C. Elbaum, J. Non-Crystalline Solids 45 (1981), 93.

"Frequency and Temperature Dependence of Ultrasonic Attenuation in the Metallic Glass $\text{Pd}_{0.775}\text{Si}_{0.165}\text{Cu}_{0.06}$ at Low Temperatures," G. Park, A. Hikata, and C. Elbaum, Phys. Rev. B23 (1981), 5597.

"Ultrasonic Attenuation in Metallic Glasses at Low Temperatures," G. Park, A. Hikata, and C. Elbaum, Phys. Rev. (1981).

"Ultrasonic Studies of Metallic Glasses at Low Temperatures," G. Park, A. Hikata, and C. Elbaum, Proceedings of the 7th Intl. Conf. on Internal Friction and Ultrasonic Attenuation in Solids, Lausanne, July 1981.

Supported by the Materials Research Laboratory NSF and the National Science Foundation.

Raman Spectroscopic Study of Molecular Orientation in Vitreous B_2O_3 Films

The presence of boroxyl rings in B_2O_3 has been widely postulated to help explain both the physical and spectroscopic properties of B_2O_3 glass, but it also has been challenged on the basis of several calculations. Our recently reported (MRL Report for 1979-80) Raman study of O- and B-isotopically substituted $\text{B}_2\text{O}_3(\text{gl})$ strongly supported the postulate of boroxyl rings within a continuous random network. We also postulated that if such interconnected boroxyl rings exist they should assume preferred orientation under tensile stress. Preferred orientation of a planar molecular unit in vitreous B_2O_3 films prepared under tensile stress has now been demonstrated by Raman spectroscopy. The polarized Raman scattering is found to be strongly dependent on sample orientation and polarization of the incident and scattered light. The ratios of scattering intensities in the various scattering arrangements for films are substantially different from those for bulk $\text{B}_2\text{O}_3(\text{gl})$. Calculated Raman intensity ratios based on the proposed oriented boroxyl ring structure compare well to the experimental values, and demonstrate the tendency of a

molecular unit with the properties of a boroxyl ring to become preferentially oriented in response to an applied stress. These results provide evidence for the existence of boroxyl rings in $B_2O_3(g)$.

Principal Investigator: W. M. Risen, Jr. (Chemistry).

Personnel: C. F. Windisch (Chemistry).

Publication: "Raman Spectroscopic Study of Molecular Orientation in Vitreous B_2O_3 Films," C. F. Windisch and W. M. Risen, Jr., *J. Noncrystalline Solids*, in press.

Supported by the Materials Research Laboratory NSF and the Office of Naval Research.

Isotopic Study of Structure in Alkali Borate Glasses

The value of using oxygen isotopic substitution in studying the structure of borate glasses was demonstrated in the Inorganic Glass group through O^{17} NMR and Raman spectra. Recently (1979-80 report) the presence of boroxyl rings in B_2O_3 was demonstrated conclusively by O^{16} , O^{18} , and O^{16}/O^{18} substitution, and the role of local structures in a demonstrably continuous random network (CRN) overall structure were investigated. This work formed the basis for determining the effect of network modification through introduction of alkali oxide. In this work Raman spectra of O^{16} , O^{18} , and mixed isotope O^{16}/O^{18} and $^{10}B/^{11}B$ glasses in the $x Na_2O(1-x)B_2O_3$ ($0 \leq x \leq 0.25$) composition range were obtained. It was shown that the introduction of alkali oxide produces new units in which vibrations are localized, as shown by the isotopic effects. In addition, the observation of bands which shift as the number-averaged isotopic weights, shows that a CRN of such units exists. These results support the boroxyl-triborate structural conversion postulate, give proof of structural localization within CRN systems, and provide data for understanding the requirements for local structure formation in glasses.

Principal Investigator: W. M. Risen, Jr. (Chemistry).

Personnel: C. F. Windisch (Chemistry).

Publication: "Raman Vibrational Study of B and O Isotopically Substituted Sodium Borate Glasses," C. F. Windisch and W. M. Risen, Jr., *J. Noncryst. Solids*, submitted, 1981.

Supported by the Materials Research Laboratory/NSF and the Office of Naval Research.

Spectroscopic Studies of Mixed Alkali Pentasilicate Glasses

The mixed alkali effect (MAE) is a special manifestation of the wide variation and continuous compositional control of both molecular level and macroscopic properties that can be achieved in inorganic glasses. It results in orders of magnitude changes as variation is carried out only in the relative composition of two alkali ion network modifiers. While the MAE ion transport phenomena was described by Risen, Rouse, and Gordon, an understanding of all related phenomena, especially including mechanical relaxation, requires thorough spectral knowledge of at least one glass system, and this is not available. The mixed alkali pentasilicate system $x Cs_2O(1-x)Na_2O \cdot 0.5SiO_2$ is the one for which most MAE data are known, and our recent Brillouin study showed that it exhibits a minimum in $K_{TO}(T_g)$ vs. x , whose interpretation can help connect the types of MAE if the ion motion spectra (far infrared) and Raman spectra are known. In this work, these spectra have been obtained as the nature of the alkali ion is varied, the value of x is varied, and the preparative and annealing conditions are controlled. It has been shown that intrinsic network strain is introduced, whose effect is a function of cation properties and x , and is manifested through Raman scattering dependence on network angles. Moreover, it was shown that two types of strain, one annealable and one intrinsic, contribute to the Raman scattering. The demonstration of intrinsic x -dependent strains permit connecting the ion transport, Brillouin, and mechanical MAE phenomena, and attempts to do so are under way.

Principal Investigator: W. M. Risen, Jr. (Chemistry).

Personnel: E. I. Kamitsos (Chemistry).

Supported by the Materials Research Laboratory/NSF and the Office of Naval Research.

O¹⁷ and H¹ NMR Studies of SiO₂

O¹⁷ and H¹ NMR spectra of amorphous SiO₂ enriched to 50% O¹⁷ have been studied. The H¹ NMR study showed that hydrogen was present in superficial hydroxyl groups which could be removed by outgassing at 500°C. Computer simulation of the O¹⁷ NMR spectrum was used to obtain the quadrupole coupling constant and the asymmetry parameter of the oxygen site. A Towns-Dailey calculation using these parameters gives charge density in the oxygen electronic orbitals which is consistent with the Si-O-Si bond angle (α) having a distribution of values ($130^\circ \leq \alpha \leq 180^\circ$), and which also weakly supports the process of π bonding between the silicon 3d and oxygen 2p orbitals. Preparation of the O¹⁷-enriched material was carried out in conjunction with Professor William Risen and his students in the Department of Chemistry.

Principal Investigator: P. J. Bray (Physics).

Personnel: A. E. Geissberger (Physics).

Publication: "Glass Structure," A. E. Geissberger, F. Bucholtz, and J. A. Harris, to appear in J. Non-Crystalline Solids.

Supported by the Materials Research Laboratory/NSF and the National Science Foundation.

B¹⁰ NMR Studies of Lithium Borate Glasses

B¹⁰ NMR studies have been carried out on lithium borate glasses over the entire glass forming region of the systems. Using the ideas of Krogh-Moe, the relative abundance of the various structural groupings was inferred from the data by fitting computer simulated lineshapes to the experimental spectra. Structural models were proposed which are consistent with the data: for $0.4 \leq R < 1.0$, where $R = \text{mol\% Li}_2\text{O/mol\% B}_2\text{O}_3$, the model states that diborate and tetraborate units are proportionately destroyed to form metaborate units and loose BO₄ units; for $1.0 \leq R < 1.86$, the model states that metaborate units and loose BO₄ units are destroyed linearly but not proportionately to form pyroborate and orthoborate units. These results have been compared with earlier B¹¹ NMR studies in this laboratory of lithium borate glasses, and agreement has been obtained.

Principal Investigator: P. J. Bray (Physics).

Personnel: W. J. Dell (Physics), S. A. Feller (Physics), and Y. H. Yun (Physics).

Publications: "B¹⁰ NMR Studies of Lithium Borate Glasses," S. A. Feller, W. J. Dell, and P. J. Bray, Bull. Am. Cer. Soc. 60 (1981) (abstract).

"B¹⁰ NMR Studies of Lithium Borate Glasses," S. A. Feller, W. J. Dell, and P. J. Bray, submitted to J. Non-Crystalline Solids.

"B¹¹ Nuclear Magnetic Resonance Studies of Li₂O-B₂O₃ Glasses at High Li₂O Content," Y. H. Yun and P. J. Bray, J. Non-Crystalline Solids 44 (1981), 227.

Supported by the Materials Research Laboratory/NSF and the National Science Foundation.

Determination of Phase Relations in the System MgO-B₂O₃ at the Metaborate Composition Using B¹¹ NMR

Using the technique of fitting computer-simulated lineshapes to experimental B¹¹ NMR spectra, it has been shown that different sample-making techniques lead to different crystalline phases in the system MgO-B₂O₃ at the metaborate composition. Sintering at 600°C leads to the formation of a mixture of magnesium diborate and unreacted magnesium oxide, while sintering at 800°C leads to the formation of a mixture of magnesium diborate and magnesium pyroborate. Melting (with or without heat treatment) leads to the formation of magnesium pyroborate and glassy boron oxide. No evidence was found for the existence of the pure metaborate compound.

In the light of these findings, models for the structure of a glass (at 44 mol% MgO) in the very narrow region of glass formation of this system have been re-examined. Using the idea of Krogh-Moe, it was concluded that the glass consists of diborate units and

boroxyl rings, that non-bridging oxygens do not exist in the glass in any significant amount, and that magnesium probably acts in part as a network former.

Principal Investigator: P. J. Bray (Physics).

Personnel: W. J. Dell (Physics).

Publications: "Determination of the Structure of Compounds and Glasses in the System $\text{MgO-B}_2\text{O}_3$ Using B^{11} NMR," W. J. Dell and P. J. Bray, *Bull. Am. Cer. Soc.* 59 (1981), 863 (abstract).

"The Determination of Phase Relations in the System $\text{MgO-B}_2\text{O}_3$ at the Metaborate Composition Using B^{11} NMR," W. J. Dell and P. J. Bray, submitted to *Physics and Chemistry of Glasses*.

Supported by the Materials Research Laboratory/NSF and the National Science Foundation.

Dependence of Glass Formation on Thermal History

The formation of glass from a melt depends on the initial temperature of the melt and the quenching rate. B^{11} NMR spectra of rapidly-quenched glass fibers have been compared with spectra obtained for slowly-cooled cullet glass of the same (commercial) composition. The results show that the fraction N_4 of four-coordinated borons in a fiber sample is approximately 10% lower than in the cullet sample. This indicates that the microstructure of the resulting glass depends on the quenching rate. Sodium borate glass of the diborate composition (33 molar % Li_2O) has also been splat-quenched between metal plates from different temperatures and studied by NMR. The B^{11} NMR spectrum for this glass sample shows no significant difference in the N_4 value of the same composition from that measured for a slowly cooled glass of the same composition. However, glasses of 10 molar % Li_2O show a reduction of N_4 by about 10% when the glass is rapidly quenched between metal plates from a melt temperature of 1000°C .

Principal Investigator: P. J. Bray (Physics).

Personnel: M. Lui (Physics).

Supported by the Materials Research Laboratory/NSF and the Owens-Corning Fiberglass Corporation.

B^{11} NMR Studies of $\text{Na}_2\text{O-B}_2\text{O}_3\text{-SiO}_2$ Glasses of High Soda and High Silica Content

Earlier B^{11} NMR data from this laboratory for this glass system at low soda-silica content were analyzed by postulating a model which states that reedmegnerite units in the glass are not destroyed by the addition of more soda; rather, non-bridging oxygens begin to form on the silicon tetrahedra. Through collaboration with S. Z. Xiao of the Beijing Glass Research Institute, People's Republic of China, we have begun to analyze this system at high soda-silica content. Preliminary NMR results indicate that the above model breaks down above a certain soda content. More complete data are being obtained and new models are being constructed to explain the coordination of the boron in these high soda, high silica glasses.

Principal Investigator: P. J. Bray (Physics).

Personnel: W. J. Dell (Physics).

Supported by the Materials Research Laboratory/NSF and the National Science Foundation.

B^{11} NMR Studies of Borate Glasses Containing Tellurium Dioxide

The nuclear magnetic resonance spectra for B^{11} in glasses of the Li_2O - TeO_2 - B_2O_3 and TeO_2 - B_2O_3 - Al_2O_3 systems were secured and used to study the behavior of N_4 , the fraction of boron atoms in four-coordination, as a function of glass composition. The appearance of non-zero values for N_4 in the TeO_2 - B_2O_3 - Al_2O_3 glasses and the enhancement of N_4 in the Li_2O - TeO_2 - B_2O_3 glasses above that obtained for the binary Li_2O - B_2O_3 glass system indicates that the TeO_2 in the glasses contributes to the formation of four-coordinated boron atoms. Models have been developed which predict the behavior of N_4 with composition in these ternary glasses. Relations describing the behavior of N_4 for the binary TeO_2 - B_2O_3 system have been inferred from the results secured for the ternary glasses.

Principal Investigator: P. J. Bray (Physics).

Personnel: I. A. Harris, Jr. (Physics).

Publications: "NMR Studies of Glass Structure," I. A. Harris, Jr., F. Bucholtz, and A. E. Geissberger. To be published in the Proceedings of the Seventh All-Union Conference on the Glassy State, Leningrad, U.S.S.R., 1981.

"NMR Studies of Glasses and Polycrystalline Materials in the System ZnO - B_2O_3 ," I. A. Harris, Jr. and P. J. Bray, *Bull. Am. Cer. Soc.* 59 (1980), 863 (abstract).

Supported by the Materials Research Laboratory/NSF and the National Science Foundation.

High Temperature Defects in Fused Silica

The equilibrium concentrations of intrinsic defects in fused silica are estimated in the temperature range 1000-2000 K, assuming that thermal Si-O bond breaking in a regular glass network creates a pair of moveable intrinsic defects: (a) 3-coordinated Si atoms and (b) non-bridging O atoms. Besides the recombination of moveable defects, which restores the regular network ($R \rightleftharpoons a + B$), two 3-coordinated Si atoms create an O vacancy ($A \rightleftharpoons a + a$) and two non-bridging O atoms create a bridging peroxy linkage ($B \rightleftharpoons b + b$). With the use of single Si-O, Si-Si, and O-O bond energies as activation energies for these reactions, the differential equations for the bridging peroxy linkage equilibrium defect concentrations are solved for different environments. There is good correlation between the temperature dependence of the equilibrium concentration of bridging peroxy linkages and the dependence of the intensity of the Raman 606 cm^{-1} mode on fictive temperatures. On this basis, bridging peroxy linkages are proposed as the source of the 606 cm^{-1} Raman mode.

Principal Investigator: P. J. Bray (Physics).

Personnel: A. R. Silin (Physics).

Publication: "High Temperature Intrinsic Defects in Fused Silica," A. R. Silin, P. J. Bray, and J. C. Mikkelsen, Jr., submitted to *J. Non-Crystalline Solids*.

Supported by the Materials Research Laboratory/NSF and the National Science Foundation.

NMR Studies of 7Li and ^{19}F in Lithium-Fluoroborate Glasses

Several fast ionic conducting lithium-fluoroborate glasses have been studied to determine whether just Li^+ , or both Li^+ and F^- ions, are responsible for the observed high conductivities. Motional narrowing studies indicate the existence of highly mobile Li ions. The Li motion appears to be governed by two activation energies, 0.03 eV and 0.2 eV. It is thought that the high local mobility of the Li ions is the result of the creation of large interstices by the anions. The motional narrowing studies are inconclusive with respect to the F ion motion; therefore, magnetic tagging experiments have been undertaken. These experiments allow an estimation of the range of ion motion through the inclusion of paramagnetic cations in the crystal lattice. Preliminary data suggest that the F ions are locally mobile with an amplitude less than 10\AA , while the Li motion at 600°K is less than 50\AA . This evidence indicates that the Li ion motion is the primary contributor to fast ionic conduction in these glasses.

Principal Investigator: P. J. Bray (Physics).

Personnel: A. E. Geissberger (Physics), F. Bucholtz (Physics), and D. E. Hintenlang (Physics).

Publications: " Li^7 , B^{11} , and F^{19} NMR in Amorphous Alkali Halogen Borate Ionic Conductors," A. E. Geissberger, F. Bucholtz, and P. J. Bray, to appear in *J. of Non-Crystalline Solids*.

"NMR Studies of the Structure of Non-Metallic Glasses," F. Bucholtz, A. E. Geissberger, and P. J. Bray, to appear in *Nuclear Instruments and Methods, Proceedings of the Intl. Conf. on Amorphous Systems Investigated by Nuclear Methods*, Balatonfured, Hungary, 1981.

Supported by the Materials Research Laboratory/NSF and the National Science Foundation.

Time Domain Spectroscopy of Glasses and Conducting Dielectrics

Previous exploratory measurements of dielectric permittivity in mixed alkali glasses revealed the presence of losses in the 10^7 to 10^{10} Hz frequency range not accounted for by ordinary conduction processes, but the measurable effects with available samples and apparatus sensitivity were too small to be determined accurately. The principal effort in the period covered by this summary was devoted to design and development of more powerful methods for these and a variety of other measurements over a wide range of frequencies above 500 KHz.

Two new systems have been designed and initially tested which have significant advantages over existing techniques. Both employ high frequency coaxial lines in bridge conformations with the bridge unbalance detected and analyzed by sampling methods, and in both it is possible to take account of all linear artifacts by calibration against precision standards. In the time domain, resolution to 10 ps and reproducibility to 1 ps has been realized; in the frequency domain, steady state measurements from 500 KHz to 250 MHz are possible with existing equipment, and a potential upper limit above 2 GHz.

With support from other sources, Paul Winsor has used the equipment to study interaction effects between ions and relaxing dipoles in conducting dielectrics. These have established the existence and importance of kinetic depolarization effects predicted by the continuum theory of Onsager and Hubbard; in the case of ions in methanol, we have found near quantitative confirmation of molecular response theory calculations by Wolynes and collaborators. Similar mechanisms of interaction are expected to operate in some glassy systems, and we hope to study these also by the new techniques.

Principal Investigator: R. H. Cole (Chemistry).

Personnel: P. Winsor IV (Chemistry).

Publications: "Molecular Correlation Function Approaches to Dielectric Relaxation," R. H. Cole, review in *Physics of Dielectric Solids*, 1980 (Conference Series 58, Institute of Physics, London).

"Electrical Response of Polymers in Solution," R. H. Cole, review in *Biological Effects of Nonionizing Radiation* (ACS Symposium Series 157, Washington, 1981).

"Dielectric Properties of Non-Aqueous Electrolyte Solutions Using Time Domain Reflectometry," P. Winsor IV, Ph.D. thesis, Brown University, 1981.

Supported by the Materials Research Laboratory/NSF and the National Science Foundation.

SECTION 4

Lower Dimensionality Materials and Structures

Introduction

Research on lower dimensionality materials and structures is directed toward both fundamental and technological aspects of the field and the participants represent a wide range of backgrounds and training. Accordingly, the contributions cover a broad spectrum of topics and investigations. The sequence in which these contributions appear on the following pages represents an attempt to order them from very general to fairly specific studies of particular systems. On the theoretical side these include the Bethe Ansatz and its relation to one- and two-dimensional models, low dimensional quantum fields and electronic disorder, properties of thin liquid crystal films, anharmonic effects in smectic liquid crystals and exchange-correlation effects in semiconducting surface space charge. On the experimental side new results are reported on valley splitting in silicon surface inversion layers as a function of surface (crystallographic) orientation, the effect of reverse substrate bias on inversion layers, and on the preparation and spectral studies of switching in the Cu-TCNQ thin film system.

SECTION 4

Lower Dimensionality Materials and Structures

Individual Contributions

Pseudo One Dimensional Conductors

Our investigation of the Bethe Ansatz has led us to conclude that, for a given internal symmetry, there is one fundamental 1D model and one Bethe Ansatz. The other 1D models are obtained from the basic one by various transformations and/or limits. This means that for every 1D model solved by a Bethe Ansatz there is a two-space dimensional (lattice) model whose transfer matrix is diagonalized by the same Ansatz. In addition to our previous results we have found that various 1D or 2D models of interest such as the Bose gas (or the XYZ-model) can be mapped onto mixed boundary value electrostatics problems. This is of particular interest in view of the emergence of electrostatics in the recent calculation of the correlation functions of the 2D Ising model (the decoupling limit of the 8V model). We believe that these methods can be applied to certain completely integrable lower dimensional systems in which there has been great recent interest. This work is continuing.

Principal Investigator: L. N Cooper (Physics).

Personnel: E. Berkcan (Physics).

Publication: "Bethe Ansatz, Periodic Boundary Conditions and Relations between Various Models," E. Berkcan, L. N Cooper, and U. Mohanty, Phys. Lett. 81A (1981), 172.

Low Dimensional Quantum Fields and Electronic Disorder

The Anderson model for localization problems has been reconsidered. We have given an exact derivation of a renormalizable field theory of interacting matrices, describing the critical behavior of the disordered electronic systems near the mobility-edge in $2 + \epsilon$ dimensions. A path-integral formulation is currently under study in order to include the effect of Coulomb-interaction between the electrons. As a first step towards a systematic treatment, Hikami and Pruisken constructed an N-orbital model, which in the limit $N \rightarrow \infty$ recovers the results previously derived in literature.

Principal Investigator: A. M. M. Pruisken (Physics).

Personnel: L. Schafer (Physics), S. Hikami (Physics), and A. Houghton (Physics).

Publications: "Field Theory and the Anderson Model for Disordered Electronic Systems," A. M. M. Pruisken and L. Schafer, Phys. Rev. Lett. 46 (1981), 490.

"The Anderson Model for Electron Localisation, Non-Linear σ -Model, Asymptotic Gauge Invariance," A. M. M. Pruisken and L. Schafer, to appear in Nucl. Phys. B.

Supported by the Materials Research Laboratory/NSF.

Thin Liquid Crystal Films

We have investigated the high-temperature behavior of a theoretical model believed to describe the smectic C-A transition in thin liquid crystal films. The molecular orientational correlation function was calculated in a formalism allowing future calculations at temperatures in the critical region. The techniques presented should also prove useful in calculating the equation of state. We have also continued a mean-field study of the order parameter behavior in these films as a function of temperature and film thickness. A simple theoretical model gives good qualitative agreement with experiment.

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Certain bulk liquid crystals (particularly smectics A and C) exhibit long-wavelength behavior characteristic of lower dimensional systems: long-range positional order is absent and correlations decay algebraically. We have studied the effects of anharmonic energy terms on the behavior of these systems. We find that conventional hydrodynamics fails and the correlation functions behave in a novel fashion. The wavevector dependence of the elastic constants predicted by this theory should prove to be experimentally measurable.

Principal Investigator: R. A. Pelcovits (Physics).

Personnel: S. Heinekamp (Physics).

Publications: "Spin-Spin Correlation Function in the High-Temperature Villain Model," R. A. Pelcovits, J. Phys. A 14 (1981), 1693.

"Anharmonic Effects in Smectic Liquid Crystals and other 'One-Dimensional Solids'," G. Grinstein and R. A. Pelcovits, Phys. Rev. Lett. 47 (1981), 856.

Supported by the Materials Research Laboratory/NSF.

Exchange-Correlation Effects in Semiconducting Surface Space Charge Layers

The possibility of a valley occupancy phase transition in silicon surface inversion layers has been studied. Exchange always favors the minimum number of valleys being occupied, in opposition to kinetic energy and correlation effects. Since all three have different density dependences, it is not clear without detailed calculation if a valley occupancy transition occurs. Sham, Bloss, and Vinter found a two-valley to one-valley transition for Si(100) surfaces. We have applied this idea to Si(111) surfaces in the hope of understanding the valley degeneracy puzzle. We have found that

- i) exchange-correlation alone cannot lead to an instability of the six-valley state for concentrations greater than $n_c \sim 5 \cdot 10^{11} \text{ cm}^{-2}$.
- ii) self-induced strain, which lowers the energy of the occupied valleys, enhances n_c but only slightly.
- iii) fairly large random uniaxial surface strains are necessary to stabilize the two-valley state at the densities up to which it is observed.

We have also studied the intersubband energies for six-valley and two-valley states with and without strains.

Principal Investigator: J. J. Quinn (Physics).

Personnel: K. S. Yi (Physics).

Publications: "Effect of Exchange-Correlation and Surface Strain on the Subband Structure of Si-(111) Inversion Layers," J. J. Quinn and K. S. Yi, Surface Science, to appear.

"Exchange Correlation Effects in Silicon (111) Inversion Layers: Stress Enhanced Valley Occupancy Phase Transition," J. J. Quinn, W. L. Bloss, and S-C. Ying, appeared in Phys. Rev. (1981).

"Properties of a Surface Inversion Layer in a Polar Semiconductor," J. J. Quinn, G. Kawamoto, and W. L. Bloss, appeared in Phys. Rev. (1981).

Supported by the Materials Research Laboratory/NSF.

Electronic Properties of Two-Dimensional Systems (EP2DS)

By studying the electronic properties of carriers in inversion (or accumulation) layers one learns of the properties of systems of lower dimensionality as well as properties of the materials and the interface. We have been heavily involved in major changes to our laboratory as well as certain experiments in the last year.

We have built a system to act as an instrumental front and rear end of all the experiments done in our laboratory. The central unit is the equivalent of a PDP 11/23 time sharing system, and controls ramp voltages, etc., and data acquisition and manipulation.

We have continued our studies of valley splitting in inversion layers in the (110) and its vicinal planes, and the (111). In addition we have completed some work on the effect of reverse substrate bias on inversion layers. The handy tool allows one to study the (EP2DS) at the same carrier density while varying the closeness to the interface, and hence separate out interface effects.

The work on the oxidation of Ge at high pressure (up to 640 Atm) has continued. This work was done almost exclusively at 550°C. We note a maximum in the dielectric constant for films grown at the 320 Atm. We are trying to construct MOSFETs now to examine fully the properties of electrons near the interface.

Principal Investigator: P. J. Stiles (Physics).

Personnel: E. Crisman (Engineering), C. Huber (Physics), J.-I. Lee (Physics), D. Syphers (Physics), K. C. Woo (Physics), and R. Zeller (Engineering).

Publications: "Effect of Reverse Substrate Bias on the Minigap in Si Inversion Layers," P. J. Stiles, T. Cole, and A. A. Lakhani, Solid State Comm. 39 (1981), 127.

"Substrate Bias Effects on Subband Separation and Interband Scattering in Si (110) p-Channel MOSFETs," P. J. Stiles, A. A. Lakhani, and T. Cole, Solid State Comm. 39 (1981), 569.

"Valley Splittings in the Valley Degeneracy Problems in Si (111) Inversion Layers," P. J. Stiles and K. C. Woo, submitted to "Comments" in PRL.

"Valley Splitting in Si Inversion Layers," P. J. Stiles and K. C. Woo, accepted for publication in the Proceedings of the 4th Intl. Conf. on EP2DS, New London, NH.

"The Oxidation of Ge Surfaces at Pressures Much Greater than One Atmosphere," P. J. Stiles, E. E. Crisman, Y. M. Ercil, and J. J. Loferski, submitted to J. Electrochem. Soc.

Supported by the Materials Research Laboratory/NSF, the National Science Foundation, and the Office of Naval Research.

Spectral Study of Switching in the Cu-TCNQ Film System

Films of TCNQ on Cu undergo an apparently electric field-induced transition from a high to low impedance state, as reported by Poehler and coworkers, and exhibit memory phenomena. The nature of the system in the unswitched (high impedance) state has been proposed to be simply $\text{Cu}^+ \text{TCNQ}^-$, while that in the switched state to be a complex pseudo-one-dimensional phase including Cu_2 and $\text{TCNQ}^{\cdot -}$ as well as Cu TCNQ salt. In order to determine both the nature of the system in these states and the reactions leading to their formation, Cu-TCNQ films were made by the reported (solution) method and by high vacuum techniques and studied by Raman and infrared spectroscopy. Pure Cu TCNQ salt was prepared and studied for reference. The Raman results show that the films prepared as reported contain Cu TCNQ, and that after switching $\text{TCNQ}^{\cdot -}$ is formed. The amount of $\text{TCNQ}^{\cdot -}$ formed by application of the field is a function of time and is related to the memory function. Conversions of from 10% TCNQ (minimum requirement to achieve low impedance) to above 40% conversion were achieved. Infrared results support the postulated transformation, although they show prior infrared reflectance data to be incorrect. The formation of thin film Cu-TCNQ devices has been achieved by vapor deposition of both Cu and TCNQ, followed by heat treatment, and demonstrated by Raman spectroscopy.

Principal Investigator: W. M. Risen, Jr. (Chemistry).

Personnel: E. I. Kamitsos (Chemistry).

Publication: "Raman Study of the Mechanism of Electrical Switching in Cu-TCNQ Films," E. I. Kamitsos and W. M. Risen, Jr., submitted to Solid State Comm., 1981.

Supported by the Materials Research Laboratory/NSF and the Office of Naval Research.

Summaries of Other Related Work

Adsorption Studies by Reflectance Spectroscopy - P. J. Estrup (Chemistry and Physics) and P. J. Stiles (Physics) - cf. Section 5.

Phase Transitions in Chemisorbed Systems - S-C. Ying (Physics) - cf. Section 5.

Electronic Properties of Surfaces and Interfaces - S-C. Ying (Physics) - cf. Section 5.

Surface Reconstruction of bcc Transition Metals - P. J. Estrup (Chemistry and Physics) - cf. Section 5.

Instantons and Disordered Systems - A. Houghton (Physics) - cf. Section 3.

SECTION 5

Solid Surfaces

Electronic Properties of Surfaces and Interfaces

The static and dynamic properties of electronic properties of low dimensional systems such as surfaces, interfaces, and point defects are being studied by a variety of theoretical techniques, such as density matrix variational method, hydrodynamics, and diagrammatic perturbation theory. New results include the response of electronic gas in different restricted geometries, electron structure around vacancies in alkali metals and effect of localization and interaction in a two-dimensional electron gas in a strong d.c. magnetic field.

Principal Investigator: S-C. Ying (Physics).

Personnel: M. Lega (Physics).

Publications: "Valley Occupancy Phase Transition in Silicon Inversion Layers," S-C. Ying, W. Bloss, and J. J. Quinn, Phys. Rev. B 23 (1981), 1839.

"Density Matrix Approach to the Study of a Monovacancy in Sodium," S-C. Ying and M. Lega, Solid State Comm. 40 (1981), 37.

"Magnetoresistance and Hall Effect of a Disordered Interacting Two Dimensional Electron Gas," S-C. Ying, A. Houghton, and J. Senna, Proceedings of the 4th Intl. Conference on Electronic Properties of Two-Dimensional Systems, New Hampshire, 1981.

"Magnetococonductance of a Disordered Interacting 2-D Electron Gas," S-C. Ying, J. Senna, and A. Houghton, Proceedings of LT-16 Conference, U.C.L.A., 1981.

"Linear Response Functions for an Inhomogeneous Electron Gas in the Hydrodynamic Approximation," S-C. Ying and F. Crowne, to appear in Phys. Rev. B.

Supported by the Materials Research Laboratory/NSF and the Navy.

Phase Transitions in Chemisorbed Systems

Both the intrinsic structural transitions of transition metal surfaces and the different phases due to adsorbate interactions in chemisorption systems are being investigated. We have paid particular emphasis in distinguishing the different behavior of long range order vs. short range order. This new understanding enabled us to resolve many apparent inconsistencies and conflicting interpretations of different experiments. A real space renormalization group scheme has been set up to study the effect of fluctuations, the global phase diagram and the dynamics of diffusion on the surface.

Principal Investigator: S-C. Ying (Physics).

Personnel: L. D. Roelofs (Physics).

Publications: "Effect of Substrate Distortion on the Ordered Phase in Chemisorption Systems," S-C. Ying, J. Vac. Sci. & Tech. 18 (1981), 500.

"Phase Transitions on W and Mo Surfaces," S-C. Ying, L. D. Roelofs, and P. Estrup, Invited Talk at the International Conference on Phase Transitions on Surfaces, Orono, 1981.

Supported by the Materials Research Laboratory/NSF.

Calculation of Phase Diagrams for Models of Surface Phase Transitions

We are considering theoretical models of phase transitions in solid surfaces. This has included simulations of lattice gas models of chemisorption systems, which has led to detailed information on the Hamiltonian governing the behavior of the system O/Ni(111). We are also considering the experimental manifestation of some features of critical phenomena, especially low-energy electron diffraction patterns and the existence of short range order. This allows close interaction with experiments by Estrup on H/W(100). For this latter system, for which we are using the model proposed by Lau and Ying (Phys. Rev. Lett. 44 (1980), 1222), we are developing a Migdal-Kadanoff renormalization group phase diagram calculation.

Principal Investigator: L. D. Roelofs (Physics).

Publications: "Diffraction from Adsorption Systems with Antiphase Boundaries or Islands," L. D. Roelofs, to appear in Surface Science Letters.

"Order in Two Dimensions," L. D. Roelofs, to appear in Applications of Surface Science.

"Monte Carlo Simulations of Chemisorbed Overlayers," L. D. Roelofs, to appear as a chapter of *Chemistry and Physics of Solid Surfaces*, published by Springer-Verlag.

Supported by the Materials Research Laboratory/NSF.

Surface Reconstruction of bcc Transition Metals

Work in this and other laboratories has shown that both clean and adsorbate-covered surfaces of transition metals may reconstruct. The conventional models of surface structures therefore must be revised. To study these problems, the (001) surfaces of tungsten and molybdenum have been investigated by LEED and associated techniques. The phase diagram for the H/W(001) adsorption system (in the region $\theta < 0.6$ monolayer, $150\text{K} < T < 450\text{K}$) has been constructed and has formed the basis for theoretical studies by Ying (see above). Several reversible phase transitions, also believed to involve substrate reconstruction, have been identified on the O/W(001) surface. Co-adsorption of H and O has been shown to produce yet another set of surface structures. Preliminary data indicate that adsorption of N_2 and CO also induce surface reconstruction of these substrates.

Principal Investigator: P. J. Estrup (Physics and Chemistry).

Personnel: A. Horlacher (Chemistry) and J-W. Chung (Physics).

Publications: "Surface Structures and Phase Diagram for the H/W(001) Chemisorption System," R. A. Barker and P. J. Estrup, J. Chem. Phys. 74 (1981), 1442.

"Surface Rearrangement of Adsorbate-Covered Mo(001)," S. Semancik and P. J. Estrup, J. Vac. Sci. Technol. 18 (1981), 541.

"Co-Adsorbed Phases of Hydrogen and Oxygen on W(001)," R. A. Barker and P. J. Estrup, J. Vac. Sci. Technol. 18 (1981), 546.

Supported by the Materials Research Laboratory/NSF and the National Science Foundation.

Experimental Studies of Chemisorption

Research has continued on the chemisorption of gaseous species on single-crystal metal surfaces. A major objective is to explore the relationship between static properties (e.g., crystallography and electronic structure) and surface kinetics. The studies employ photo- and Auger-electron spectroscopy, mass spectrometry, surface reflectance spectroscopy (SRS), and LEED.

The rate of isothermal dissociation of molecules adsorbed on Mo and W has been measured by continuously monitoring the UPS and AES spectra. Contrary to expectation, the dissociation of CO on Mo is not unimolecular. The activation energy is ~ 0.6 eV at low coverage but rises sharply when the substrate, according to LEED and SRS, undergoes structural changes. The decomposition of ethylene on W also shows complex kinetics. On the (001) plane the activation energy is ~ 0.9 eV but the

rate depends strongly on the substrate structure and composition. Thus, co-adsorption of oxygen raises the activation energy by 50%.

Principal Investigator: P. J. Estrup (Physics and Chemistry).

Personnel: J. Erikson (Chemistry), S. Semancik (Physics), and J. Prybyla (Chemistry).

Publications: "The Kinetics of CO Dissociation on Mo(001)," S. Semancik and P. J. Estrup, *Surface Science* 104 (1981), 26.

"Hydrogen on Transition Metals," J. Davenport and P. J. Estrup, in *The Chemical Physics of Solid Surfaces*, to be published.

Supported by the Materials Research Laboratory/NSF.

Adsorption Studies by Reflectance Spectroscopy

A method for the analysis of surface reflectance spectroscopy (SRS) data has been developed and applied to hydrogen chemisorbed on tungsten (110). The main features of the reflectance spectrum have been calculated for different structural models and a comparison with experiments shows that the most likely adatom position is in a bridged site. In addition, the location of the resonance levels and adsorbate states in the surface band structure have been determined.

Reflectance spectroscopy has also been used to investigate overlayers of chemisorbed oxygen on tungsten (110). The work has demonstrated that the two-dimensional phase transitions occurring in this system are accompanied by characteristic changes in the surface electronic properties and, therefore, can be studied by SRS. The phase boundaries in the temperature-coverage plane, obtained by SRS, agree well with previous LEED results but the spectral dependence of the reflectivity changes suggests the need for improved structural models of the surface phases.

Principal Investigators: P. J. Estrup (Physics and Chemistry) and P. J. Stiles (Physics).

Personnel: G. B. Blanchet (Physics).

Publications: "A Study of the H/W(110) Adsorption System by Surface Reflectance Spectroscopy," G. B. Blanchet, P. J. Estrup, and P. J. Stiles, *Phys. Rev. B* 23 (1981), 3655.

"SRS Studies of the O/W(110) Phase Diagram," G. B. Blanchet, P. J. Estrup, and P. J. Stiles, *J. Vac. Sci. Technol.* 18 (1981), 502.

Supported by the Materials Research Laboratory/NSF.

Surface Reflectance Spectroscopy (SRS)

Our previous experience in studying metal surfaces by SRS indicates that this method can be extended to investigations of surfaces of semiconductors such as Si and Ge. In order to accomplish this, a series of modifications of the equipment has been undertaken. The sample mounting has been moved to a carousel in the middle of the vacuum chamber where cleaning by ion bombardment, and monitoring by Auger spectroscopy and LEED, can be performed. In addition, equipment is being constructed to allow the application of a large electric field perpendicular to the surface so that electroreflectance measurements may become feasible.

Principal Investigator: P. J. Stiles (Physics).

Personnel: B. D. Parker (Physics).

Supported by the Materials Research Laboratory/NSF.

Models of Surface Complexes at Pt Centers in PFSA Ionomers

Studies of reactions of small molecules with metal atom clusters or metal ions supported in PFSA ionomers and of the interactions between the metals and the ionomeric support are designed to help develop an understanding of the structure and bonding of chemisorbed species on supported metals or ions at surface sites. Our work on reactions of the Rh-PFSA system with CO and H₂ established a clear connection between these systems and those, such as CO on Rh supported on inorganic oxides, known to be catalytic. In this year Pt-PFSA systems, with Pt(II) incorporated into ionic domains of PFSA-ionomers, have been achieved by both exchange with tetraamine-platinum(II) and domain-mediated growth of PtCl_{2-x}(OH)_x(H₂O)_n species. Reactions with CO, H₂ and isotopically labelled forms of them have been carried out. Initially two types of adsorbed CO, one π -chemisorbed and one physisorbed, were found, and upon thermal treatment, Pt(O) clusters were formed, and CO on Pt⁰ was observed. Reduction was achieved by H₂ of CO on hydrated Pt-PFSA and production of CO₂ was confirmed isotopically, so the use of this in the gas shift reaction is demonstrated. Reactions with CO, H₂, and C₂H₂ were carried out and resulted in identification by infrared of a Pt⁰ species with both C₂H₂ and CO chemisorbed.

Principal Investigator: W. M. Risen, Jr. (Chemistry).

Personnel: S. U. Noor (Chemistry).

Publication: "Chemisorption Studies of Small Molecules on Platinum Nafion," S. U. Noor and W. M. Risen, Jr., J. Catal., in submission, 1982.

Supported by the Materials Research Laboratory/NSF and the Office of Naval Research.

The Scattering and Ionization of Atoms at Surfaces

Measurements of the efficiency of the formation of ions when thermal atoms of K, Na, Li, and Tl hit silicon surfaces are being interpreted to yield detailed information about the interaction of the atoms with the surface. The quantities determined are the work function of the surface and several characteristics of the adsorbed species. The latter include the residence time, the energies of desorption to ions and to atoms, the rate of diffusion on the surface, and the cross section for desorption as the result of collision with other adsorbed species.

A completely redesigned and rebuilt apparatus for the study of the elastic and nearly elastic scattering of rare gases from crystalline surfaces has been completed and is being tested. The first system to be studied will be Ar scattered from the (0001) plane of graphite.

Principal Investigator: E. F. Greene (Chemistry).

Personnel: A. LeGrand (Physics), J. Keeley (Chemistry), and M. Pickering (Chemistry).

Supported by the U.S. Department of Energy and the Materials Research Laboratory/NSF.

Inelastic Scattering of Diatomic Molecules on Solid Surfaces

We have completed experiments that demonstrate the feasibility of detection of the momentum flux in atomic and molecular beams scattered from solid surfaces. The sensitivity of the detector has been found to correspond to 1×10^6 atoms/cm³ for an effusion argon beam when the detector is operated at room temperature.

At the same time we are continuing experiments with cooled beams of NO scattered from solid surfaces with laser induced multiphoton ionization as a probe of the final state distribution. We have succeeded in cooling the incident beam to a few degrees Kelvin through the use of high pressure seeded beams produced in a short pulse (50 μ s) valve.

Rotational distributions are measured by focusing the output from a tunable dye laser into the scattering chamber near the target. The laser is tuned to the C-X transition in NO (via a two photon transition) so that a third photon ionizes NO to NO⁺. The multiphoton ionization technique has been shown to be much more sensitive than fluorescence detection from the A or C state

and yet still provides the required state sensitive detection. Ions are collected with a channeltron and the resulting signal is processed with a boxcar averager. Experiments to measure the degree of equilibration of rotation with the surface are still in progress.

Principal Investigator: G. J. Diebold (Chemistry).

Personnel: J. S. Hayden (Chemistry).

Publication: "Direct Detection of Momentum Flux in Atomic and Molecular Beams," J. S. Choi, J. S. Hayden, M. T. O'Connor, and G. J. Diebold, J. Appl. Phys. 52 (1981), 6016.

Supported by the Materials Research Laboratory/NSF and the Petroleum Research Fund.

Summary of Other Related Work

Exchange-Correlation Effects in Semiconducting Surface Space Charge Layers - J. J. Quinn (Physics) - cf. Section 4.

SECTION 6

Properties of Materials at Low Temperatures

Second Sound and Heat Flow in Anisotropic Solids

The solids in which second-sound can be most readily observed are solid ^4He and bismuth, both of which are anisotropic elastically. We have studied the effects of anisotropy on second sound propagation and have succeeded in showing for the first time that even in anisotropic crystals the heat flux vector and the phonon drift velocity are in the same direction. This enables us to derive a simple closed-form expression for the second-sound velocity as a function of propagation direction.

Principal Investigator: H. J. Maris (Physics).

Publication: "Second Sound and Heat Flow in Anisotropic Solids," H. J. Maris, Phys. Rev. B 24 (1981), 1205.

Supported by the National Science Foundation.

Properties of the Interface Between Liquid and Solid Helium-4

The interface between liquid and solid ^4He at low temperatures has unique properties. Andreev and Parshin have proposed that because of quantum delocalization effects the boundary should be in a special state which may be regarded as a quantum analog of an atomically rough surface. Under these conditions melting and freezing at zero temperature takes place in a reversible way without dissipation. Castaing and Nozieres have shown that this rapid melting and freezing (RMF) leads to a greatly reduced transmission of sound and phonons across the interface. We have observed this effect experimentally using phonons of frequency in the range 10^{10} to 10^{11} Hz. In this way we are able to show that melting and freezing in this system can occur in a coherent reversible way even on time scales as short as 10^{-11} secs. These results provide a striking confirmation of the Andreev-Parshin theory.

Principal Investigator: H. J. Maris (Physics).

Personnel: T. Huber (Physics).

Publication: "Capillary Effects on the Phonon Transmission Between Liquid and Solid Helium," T. E. Huber and H. J. Maris, Phys. Rev. Lett., to appear December 1981.

Supported by the National Science Foundation.

Ultrasonic Attenuation and Plastic Deformation in Solid Helium-Four

We have studied the changes in ultrasonic attenuation of plastically deformed helium-four crystals subjected to rapid compression or decompression, with a resulting length change of 0.05 to 0.1%. It was thus found that as a result of the strain the ultrasonic attenuation first increased in a time comparable to that involved in the change of length (several seconds). The attenuation subsequently returned to the original value with a time constant of about ten minutes. Throughout this decay the attenuation varied quasi-periodically in time with a period of about one minute (up to six "oscillations" were observed). The behavior of the attenuation displays features of an interference phenomenon between waves reflected from two interfaces. Further studies of this phenomenon will be carried out.

Principal Investigator: C. Elbaum (Physics and Applied Mathematics).

Personnel: A. Hikata (Applied Mathematics).

Supported by the Materials Research Laboratory/NSF and the National Science Foundation.

Heat Transport in Dielectric Glasses

The temperature dependence of the thermal conductivity of essentially all dielectric glasses (and other amorphous materials) shows a "plateau" between 1 and 10 K. There is currently no theoretical explanation of this effect. To increase the understanding of phonon propagation in this temperature range, we have begun to make measurements of the conductivity of samples of amorphous germanium in restricted geometries.

Principal Investigator: H. J. Maris (Physics).

Personnel: M. Williams (Physics).

Supported by the National Science Foundation.

Properties of Atomic Hydrogen at Low Temperature

ESR measurements have been performed on atomic hydrogen below 1°K. To reduce the problems of rapid recombination of H atoms in contact with walls below 4.2°K not coated with a helium film we have constructed an orifice in the connecting tube transporting the hydrogen from high to low temperatures. This geometry creates an abrupt temperature change in the tube wall from 4°K to 0.6°K, the low temperature section being coated with a saturated superfluid film of helium. The film flow is restricted by the orifice and the heat is kept small from the recondensing He gas to the dilution refrigerator used to maintain temperatures below 1°K.

The H atoms have been detected both calorimetrically as well as by ESR. On turning off the source of atomic hydrogen, the density of atoms in the low temperature cavity is observed to decay exponentially with a time constant in excess of 250 sec. This relatively long time constant in a field and temperature regime where magnetic confinement is not important is due to the orifice geometry and to the pumping action of the refluxing He gas. At higher densities ($3 \times 10^{15}/\text{cm}^3$) the decay in the number of H atoms is markedly nonexponential, and is found to be described well mathematically by three-body recombination. Preliminary measurements indicate that to the accuracy of our density determinations of both H and He, the rate constant for three-body recombination is somewhat smaller than expected. Relaxation time measurements are consistent with the predictions of spin exchange.

Principal Investigator: G. Seidel (Physics).

Personnel: R. Mayer (Physics) and J. Cameron (Physics).

Publication: "ESR Experiments on Atomic Hydrogen," R. Mayer, A. Ridner, and G. Seidel, Physics B-C 107 (1981), 937.

Supported by the Materials Research Laboratory/NSF and the National Science Foundation.

SECTION 7

Materials for Solar Energy Conversion

Photoelectrolysis

Preparation and Properties of the Systems $\text{Fe}_{1-x}\text{V}_x\text{NbO}_4$ and $\text{Fe}_{1-x}\text{Cr}_x\text{NbO}_4$

Members of the system $\text{Fe}_{1-x}\text{V}_x\text{NbO}_4$ were prepared and their crystallographic, electrical, and magnetic properties were determined. The wolframite structure is formed for $x \leq 0.2$ but for $x \geq 0.4$, a phase transition to the rutile structure takes place. Magnetic studies established the formal valences of the elements for members crystallizing with the wolframite phase. However, similar analyses of compounds with the rutile structure did not provide a unique assignment of the formal valences.

For the system $\text{Fe}_{1-x}\text{Cr}_x\text{NbO}_4$, it was shown that chromium substitution favored the formation of the rutile structure, which resulted in a decrease in the electrical conductivity because of randomization of the transition metal ions in the structure. The replacement of a few percent of Fe^{3+} with Cr^{3+} caused a significant lowering of the lowest optical band gap, whereas the higher-energy transitions remained essentially unchanged. This resulted in increased response to the longer wavelengths of the solar spectrum.

Preparation and Characterization of Conducting Iron Tungstates

Several iron(III) tungstates have been prepared, and their crystallographic, magnetic, electric, and photoelectronic properties have been characterized. The compounds crystallized with the tri- α - PbO_2 structure, and the actual ordering of the MO_6 octahedra ($M = \text{Fe}$ or W) appears to determine these properties. Under illumination, Fe_2WO_6 photoanodes show an intermediate photo-response between conducting α - Fe_2O_3 and WO_3 , although the flat-band potential is still too positive.

Principal Investigator: A. Wold (Chemistry).

Personnel: See below (Hydrodesulfurization Catalysts).

Publications: See below (Hydrodesulfurization Catalysts).

Hydrodesulfurization Catalysts

The Preparation and Properties of the Systems $\text{Co}_{1-x}\text{Rh}_x\text{S}_2$ and $\text{Co}_{1-x}\text{Ru}_x\text{S}_2$

Members of the systems $\text{Co}_{1-x}\text{Rh}_x\text{S}_2$ ($0 \leq x \leq 0.6$) were prepared and their crystallographic and magnetic properties were studied. The observed ferromagnetic moments for compositions where $x \leq 0.2$ indicate a ferromagnetic alignment between $\text{Co}(3d^7)$ and $\text{Rh}(4d^7)$ electrons. For larger concentrations of rhodium, there is a reduction in the observed moment which can be attributed to a lack of magnetic homogeneity in these samples with the possible formation of rhodium clusters. The paramagnetic data are consistent with results obtained in the ferromagnetic region.

For members of the system $\text{Co}_{1-x}\text{Ru}_x\text{S}_2$ ($0 \leq x \leq 1$), the Curie points increased initially with increasing ruthenium concentration and then decreased. This is indicative of an initial decrease in antiferromagnetic interactions followed by a decrease in all magnetic interactions.

Principal Investigator: A. Wold (Chemistry).

Personnel: K. Dwight (Chemistry), R. Kershaw (Engineering), J. Hornadaly (Chemistry), K. Kim (Chemistry), R. Kaner (Chemistry), J. Koenitzer (Chemistry), H. Leiva (Chemistry), J. Passaretti (Chemistry), V. Nguyen (Chemistry), B. Khazai (Chemistry), R. Chianelli (Exxon Research and Engineering), and W. Croft (Chemistry).

Publications: "The Preparation and Characterization of Materials," A. Wold, J. Chem. Education 57 (1980), 531.

"Preparation and Photoelectronic Properties of FeNbO_4 ," J. Koenitzer, B. Khazai, J. Hormadaly, R. Kershaw, K. Dwight, and A. Wold, *J. Solid State Chemistry* 35 (1980), 128.

"Oxyfluoride Photoelectrodes for the Photodecomposition of Water by Solar Energy," A. Wold and K. Dwight, *Advances in Chemistry Series No. 186 Solid State Chemistry: A Contemporary Overview*, ACS (1980), 161.

"Photoelectronic Properties of Ternary Niobium Oxides," K. Dwight and A. Wold, *ACS Symposium Series no. 146*, ACS (1981), 207.

"Synthesis of Poorly Crystallized Platinum Metal Dichalcogenides," J. Passaretti, R. Kaner, R. Kershaw, and A. Wold, *Inorganic Chemistry* 20 (1981), 501.

"Conductivity as a Tool for Evaluating the Homogeneity of Sintered Discs of Transition Metal Oxides," R. Kershaw, B. Khazai, H. Leiva, K. Dwight, and A. Wold, *Mat. Res. Bull.* 16 (1981), 335.

"Preparation and Photoelectronic Properties of the System $\text{Cd}_2\text{Ge}_{1-x}\text{Si}_x\text{O}_4$," V. Nguyen, R. Kershaw, K. Dwight, and A. Wold, *J. Solid State Chemistry* 36 (1981), 241.

"Preparation and Properties of the System $\text{Fe}_{1-x}\text{V}_x\text{NbO}_4$," B. Khazai, R. Kershaw, K. Dwight, and A. Wold, *J. Solid State Chemistry* 39 (1981), 294.

"Preparation and Properties of the System $\text{Fe}_{1-x}\text{Cr}_x\text{NbO}_4$," B. Khazai, R. Kershaw, K. Dwight, and A. Wold, *J. Solid State Chemistry* 39 (1981), 395.

"Preparation and Properties of Several Members of the System $\text{Fe}_x\text{Nb}_{2x/3}\text{Ti}_{1-x}\text{O}_2$," B. Khazai, R. Kershaw, K. Dwight, and A. Wold, *Mat. Res. Bull.* 16 (1981), 655.

"Preparation and Properties of Poorly Crystallized CoS_2 and RuS_2 ," J. Passaretti, K. Dwight, A. Wold, W. Croft, and R. Chianelli, *Inorganic Chemistry* 20 (1981), 2631.

"Preparation and Properties of Members of the Co-S System Close to Co_9S_8 ," K. Kim, K. Dwight, and A. Wold, *Mat. Res. Bull.* 16 (1981), 1319.

Supported by the Materials Research Laboratory/NSF, the National Science Foundation, the Office of Naval Research, the Solar Energy Research Institute, and the Exxon Research and Engineering Company.

Investigations of Photovoltaic Solar Cells

Our work during this year has continued to focus primarily on solar cells based on ternary chalcopyrite semiconductors like CuInSe_2 and their alloys like $\text{CuIn}_{1-y}\text{Ga}_y\text{Se}_{2z}\text{Te}_{2(1-z)}$, but has also included germanium based photovoltaic cells intended for thermophotovoltaic (TPV) applications. In the TPV application the PV cells are exposed to a radiation source consisting of a mantle heated to incandescence by focusing sunlight onto the absorber.

The ternary chalcopyrite program began in 1977. It has as its goal the fabrication of thin film heterojunction solar cells in which one of the semiconductors is n-CdS and the other, the photovoltaically active semiconductor (PVAS), is CuInSe_2 or an alloy of CuInSe_2 with other I-III-VI₂ semiconductors. We have continued producing ternary films by rf-sputtering from targets of compressed, previously synthesized powders having the desired composition. During this year, we have been mainly concerned with CuInSe_2 as the PVAS. The films are characterized by a four point probe for typeness and resistivity; by an EDAX system for composition; by x-ray diffraction for structure; by a spectrophotometer for optical transmission, and by an SEM for morphology. As reported last year, we can deposit with reasonable reproducibility films that are p-type; have resistivities in the 1 to 10 ohm-cm range; have grain sizes of about 1 μm ; are stoichiometric within the measurement capability of the EDAX system and have the chalcopyrite x-ray diffraction pattern. These CuInSe_2 films are covered by low resistivity (<0.1 ohm-cm) CdS films produced by rf-sputtering and/or evaporation from a resistance heated crucible. The CdS powder used for evaporation and for the sputtering targets is heated in pure hydrogen to produce a CdS powder containing excess Cd. We have established evaporation conditions which result in CdS films having a resistivity of the order of 0.01 ohm-cm when deposited onto CuInSe_2 substrates maintained at $T_{\text{substrate}}$ about 200°C. For such low substrate temperatures, CdS films having such a low resistivity have previ-

ously been produced only by doping the CdS with large amounts ($\sim 1\%$) of indium. Solar cells made from our Cd-rich CdS and the rf-sputtered films have exhibited efficiencies up to about 5%. Analysis of the i-V characteristics of the cells indicates an excessive series resistance which we attribute to the sheet resistance of the CdS; we hope to reduce this series resistance by depositing a transparent conducting coating like indium-tin oxide over the CdS. Our ohmic contact grid lines cover about 30% of the area of the cells; by resorting to finer grid lines, we expect to reduce the coverage to about 10% and thereby further increase efficiency. These two losses may account for a total reduction in cell efficiency of about 30%, i.e., our 5% cells may in fact be 6.5% cells.

We have also begun fabrication of cells incorporating the minority carrier mirror (MCM) concept whose beneficial effect is predicted by a theoretical study reported in last year's MRL report. An MCM is an electrostatic barrier which prevents the flow of minority carriers away from the charge collecting barrier of the cell (e.g., the p-n junction). The particular MCM we are fabricating is the barrier between a P⁺-type film of $\text{CuGaSe}_{0.9}\text{Te}_{0.1}$, which has $E_G \sim 1.4$ eV, and a p-type CuInSe_2 film. This MCM contains both favorable resistivity and band gap profiles.

Our study of Ge PV cells has been concerned with passivation of the surfaces of the Ge PV cells. This work has involved the growth of thick (several thousand Angstroms) native oxide layers on Ge crystals by high pressure oxidation. The oxide serves as a wide band gap window which admits light to the Ge. Estimates of the interface recombination velocity s_i of Ge PV cells with and without the oxide coating, as determined from analyses of PV spectral response curves, have shown that there is a considerable reduction of s_i in oxide coated cells. This is consistent with our finding that the interface generation velocity s_g for such a Ge-Ge oxide interface is extremely low. These s_g values were determined from analyses of transient capacitance curves of MOS devices made from oxide covered Ge crystals.

We have extended our theoretical calculations of cell performance to include materials having the band gaps 1.25, 1.35, and 1.45 eV since we have been producing alloys having these values of energy gap. The calculations have included reflection and absorption losses in the CdS overlayer which were based on measured absorption and reflection curves of our CdS films. The larger band gap materials have a slight efficiency advantage over CuInSe_2 ; they are of special interest to us as potential building blocks of monolithic tandem solar cells.

Principal Investigators: J. J. Loferski (Engineering) and B. Roessler (Engineering).

Personnel: A. Bouazzi (Engineering), G. Kenshole (Engineering), T. Warminski (Engineering), M. Kwietniak (Engineering), E. Crisman (Engineering and Physics), B. Agbara (Engineering), R. Beaulieu (Engineering), J. Sachs (Engineering), W. Oates (Engineering), P. Sarro (Engineering), R. Arya (Engineering), D. Burk (Engineering), C. Case (Engineering), G. Doodlesack (Engineering), Y. Ercil (Engineering), C. Toro (Engineering), M. Spitzer (Physics), E. Vera (Physics), and L. Susani (Engineering).

Publications: "Grating-Type Si Solar Cell Design and Analysis," H. L. Hwang, D. C. Liu, Y. L. Yen, and J. J. Loferski, Proceedings of the 15th IEEE Photovoltaic Specialists Conference, Orlando, Florida, June 1981, pp.883-87.

" $\text{Cu}_2\text{S}/\text{CdS}$ Solar Cells Prepared by Organometallic Chemical Vapor Deposition: Preliminary Stage," H. L. Hwang, J. S. Ho, Y. K. Lee, C. Y. Sun, C. J. Chen, and J. J. Loferski, Proceedings of the 15th IEEE Photovoltaic Specialists Conference, Orlando, Florida, June 1981, pp.1035-40.

"A Brief Summary of Research at Tsing Hua on CuInS_2 —A New Photovoltaic Material," H. L. Hwang, C. Y. Sun, H. M. Yang, C. R. Chen, L. M. Liu, B. H. Tseng, and J. J. Loferski, Proceedings of the 15th IEEE Photovoltaic Specialists Conference, Orlando, Florida, June 1981, pp.1277-82.

"Current from the Sun—A Look at the Economics of Solar Cells," J. J. Loferski, The Sciences (July/August 1980), 6-9, 29.

"Solar Cell Research and Development—Future Trends," J. J. Loferski, Proceedings of the First Republic of China's Solar Cell Workshop, Hsin-Chu, Taiwan, R.O.C., October 1980, pp.77-86.

"Research Options As Seen From U.S.A.," J. J. Loferski, Proceedings of the 3rd International Photovoltaic Solar Energy Conference, Cannes, France, October 1980, pp.194-98.

"Keynote Address—Photovoltaics 1981 and Future Prospects," J. J. Loferski, Proceedings of the 15th IEEE Photovoltaic Specialists Conference, Orlando, Florida, June 1981, pp.1-3.

"Thin Film Heterojunction Solar Cells Based on n-CdS and p-Cu Ternary Alloys of the Type $\text{CuInGa}_{1-x-y}\text{Se}_{2z}\text{Te}_{2(1-z)}$," J. J. Loferski, M. Kwietniak, J. Piekoszewski, M. Spitzer, R. Arya, B. Roessler, R. Beaulieu, E. Vera, J. Shewchun, and L. L. Kazmerski, Proceedings of the 15th IEEE Photovoltaic Specialists Conference, Orlando, Florida, June 1981, pp.1056-61.

"Measurement of Diffusion Length in CuInSe_2 and CdS by the Electron Beam Induced Current Method," J. M. Piekoszewski, L. Castaner, and J. J. Loferski, J. Appl. Phys. 70 (1980), pp.5375-79.

"Combined Photovoltaic Thermal Collector Panels of Improved Design," T. Russell, J. Beall, J. J. Loferski, B. Roessler, R. Dobbins, J. Shewchun, J. Krikorian, C. Case, G. Doodlesack, and W. Oates, Proceedings of the 15th IEEE Photovoltaic Specialists Conference, Orlando, Florida, June 1981, pp.990-96.

"Performance of Ultra High Efficiency Thin Germanium P-N Junction Solar Cells Intended for Solar Thermophotovoltaic Application," E. S. Vera, J. J. Loferski, M. Spitzer, and J. Shewchun, Proceedings of the 3rd International Photovoltaic Solar Energy Conference, Cannes, France, October 1980, pp.911-19.

"Theoretical Limit Efficiency of Two Junction Tandem Silicon-Germanium Solar Cells Intended for Thermophotovoltaic Application," E. S. Vera, J. J. Loferski, and M. Spitzer, Proceedings of the 15th IEEE Photovoltaic Specialists Conference, Orlando, Florida, June 1981, pp.877-82.

Supported by the Materials Research Laboratory/NSF, the Solar Energy Research Institute, the U.S. Department of Energy, Amperex Corporation, New England Electric System, and the Naval Research Laboratory.

Semiconductor Powder Processing for Photovoltaic Cells

This program was initiated midway in the year. It is concerned with the fabrication and characterization of large grained compacts of alloys of the copper ternary semiconductors like CuInSe_2 , CuInS_2 , etc. The potential of these materials for the fabrication of extremely low cost photovoltaic cells is high, since conversion efficiencies of 9.5% have been achieved by other investigators using them in photovoltaic cells with CdS. Moreover, they appear to be remarkably stable or even to improve with time during use and/or storage. Our initial work on this program has been concerned primarily with the design and construction of a cathodoluminescent attachment for the AMR scanning electron microscope in the Brown MRL Electron Microscopy Facility. The initial design work has been completed and several of the required components obtained. Progress on the construction has been delayed by the deferral of Visiting Professor T. Warminski's arrival from the Polish Academy of Sciences until the summer.

The cathodoluminescent attachment, which is the major focus of our attention during the initial stages of this program, is to be used for characterization work on the semiconductor materials being used in this program, as well as others, for fabrication of solar cells. It should provide a large improvement in the cathodoluminescent signal from specimens being examined for localized and overall homogeneity and structure. Previous work showed that the signal strength, using equipment supplied by the manufacturer of our SEM, was inadequate for our purposes. We have, therefore, designed a device whose main optical component is a half-ellipsoidal mirror; the specimen to be examined is located at one focus and a lens and fiber optical bundle at the other. The cathodoluminescent signal which is generated in synchronism with the scanning electron beam is passed through the vacuum chamber to an external grating monochromator for wavelength analyses of the cathodoluminescence. It is expected that, when adequately cooled, localized variations in wavelength (and energy gap) can be observed. This system, therefore, should be invaluable as a means of assessing homogeneity and structure in terms of parameters (E_g) of direct concern in fabrication of cells. Construction of the equipment will take place during the next year's program. Characterization work using SEM, microprobe, EDAX, and resistivity and typeness are continuing as background data in connection with the other programs in this area.

Principal Investigators: B. Roessler (Engineering), J. J. Loferski (Engineering), and J. Gurland (Engineering).

Personnel: T. Warminski (Engineering), M. Kwietniak (Engineering), U. Schwuttke (Engineering), P. Delzio (Engineering), and W. Oates (Engineering).

Supported by the Materials Research Laboratory/NSF.

Summary of Other Related Work

X-Ray Typography - B. Roessler (Engineering) - cf. Section 8.

SECTION 8

Other Research

Covalent Bonding in Polymers

In recent years, two distinct approaches to the modelling of the strong covalent bonds in chain molecules have been distinguished and studied. They lead to what are generally referred to as rigid and flexible models, and the terminology describes two methods for the computation of the model partition function.

For a rigid model, strong covalent bonds are modelled by geometric constraints (such as fixed bond lengths and fixed valence angles) in the Hamiltonian H_r of the model, which must therefore be written in terms of suitable generalized coordinate s . The partition function for the rigid model, Z_r , is then computed on the basis of H_r .

In a flexible model, the strong covalent bonds are modelled first by stiff linear springs whose spring constant is scaled by a parameter κ . Since there are no geometric constraints, the Hamiltonian H_f can be expressed either in terms of rectangular Cartesian coordinates or in terms of a set of convenient curvilinear coordinates. The partition function for the flexible model, Z_f , is then computed on the basis of H_f . Finally, the spring-constant scaling factor is regarded as arbitrarily large.

We have considered the force-length-temperature relation in short stretched polymers based on the two types of models. For the two-bond freely-jointed chain, the two models give completely different results. As the number of bonds increases, the behavior of the two approaches coincidence. The above analysis has been purely classical. We have also treated the high-frequency modes associated with the covalent bonds of the flexible model on the basis of quantum statistical mechanics. It is found that at 300°K the quantum force-length-temperature relation is almost identical to the classical flexible model result. The quantum analysis at low-temperature levels does not approach the classical rigid-model predictions because the zero-point energy is deformation-dependent.

Principal Investigator: J. H. Weiner (Engineering).

Personnel: D. Perchak (Physics) and T. Stevens (Engineering).

Publications: "Classical and Quantum Calculations for Short Stretched Chain Models," D. Perchak and J. H. Weiner, submitted to *Macromolecules*.

"Use of $S = k \log p$ for Stretched Polymers," J. H. Weiner, submitted to *Macromolecules*.

Supported by the Materials Research Laboratory/NSF and the Gas Research Institute.

X-Ray Topography

The experimental portion of the research on studies of oxidation in zinc by x-ray topography and the correlation with surface features has been completed. Observations of the crystal surface by scanning electron microscopy, microprobe, and optical and Nomarski interference microscopy and of microprobe measurements of oxygen and zinc x-ray intensities have clarified the details of the correlation.

The use of the Nomarski interference equipment purchased by the MRL for use on this and related programs has been extremely helpful in indicating the locations on the surface at which thermal etch pits occur. These pits appear to locate the termination point of dislocations that have climbed to the surface as a result of vacancy injection into the lattice during the oxidation process. Berg-Barrett x-ray topographs do not generally show such features, but instead reveal portions of the dislocation network which are present beneath the crystal surface and are roughly parallel to it. The piercing or termination points appear, therefore, to provide the vacancy short circuit path for vacancy injection and climb and thus confirm the models previously advanced. Several new features of the climb-oxidation processes associated with the presence and the change in spiral loop dislocations have been clarified by use of three-dimensional, i.e., stereo Berg-Barrett topography—a technique developed for

this purpose. In particular, the dislocation spirals are now seen to be bundles of assorted slip dislocations and the contrast effects in x-ray topographs indicate the Burgers vectors of the constituent dislocation groups. Hexagonal pits on the surface, when sufficiently developed by oxidation, coincide with the images in x-ray topographs. A dislocation model for the development of spirals by slip around obstacles and elastic interaction has also been deduced on the basis of the topographic results.

In addition to the work on oxidation, a cooperative program with the National Bureau of Standards on x-ray topography was begun during the summer. This included a visit for two months during the summer as a guest at NBS by K. C. Yoo and by B. Roessler for several days. This work was concerned with planning and design of experimental work on synchrotron radiation topography and with Berg-Barrett studies by conventional means of the plastically deformed regions near hardness impressions in copper single crystals. This work was completed in October and a publication on it prepared.

Principal Investigator: B. Roessler (Engineering).

Personnel: K. C. Yoo (Engineering) and W. Oates (Engineering).

Publications: "Reflection X-Ray Topography of Hardness Indentations in Copper Single Crystals," K. C. Yoo, B. Roessler, R. W. Armstrong, and M. Kuriyama, submitted to Scripta Metallurgica.

"Study of Oxidation Processes in Metals by X-Ray Topography and Scanning Electron Microscopy," K. C. Yoo, prepared for and submitted to Center for Materials Science, National Bureau of Standards, 1980.

Supported by the Materials Research Laboratory NSF and the National Bureau of Standards.

Highly Excited Electronic States on Semiconductors

Picosecond pulse infrared laser techniques have been applied to probe the dielectric properties and the kinetics of dense nonequilibrium electron-hole systems in narrow-gap semiconductors including InSb, Hg, CdTe, and PbTe. Specifically, time resolved luminescence together with picosecond probe transmission and reflectivity measurements have been used to examine intraband and interband contributions of the highly degenerate electron-hole system. As an example of our results, large optical gains at near bandgap energies have been measured in PbTe with accompanying luminescence of surprising intensity. The luminescence spectrum is unexpectedly narrow and shows features more typical of amplified spontaneous ("superradiant") emission. In contrast, narrow-gap materials of zinc-blend symmetry show little evidence of luminescence but rather the prevalence of nonradiative (Auger) recombination. Such processes have nevertheless been found to scale rather slowly with increasing density, apparently due to screening effects in the degenerate carrier gas. The work is presently continuing with emphasis on study of the role of electron-hole correlations on the optical transition strengths and the construction of ultrashort resonator semiconductor lasers.

Principal Investigator: A. V. Nurmikko (Engineering).

Personnel: J. Ajo (Engineering).

Publications: "Picosecond Spectroscopy of Highly Excited Electronic States in Narrow-Gap Semiconductors," A. V. Nurmikko and B. D. Schwartz, J. Phys. Soc. Japan 49 (1980), 511, Proc. of 15th Intl. Conf. Physics of Semiconductors

"Optical Studies of a High Density Electron-Hole Plasma in PbTe," B. D. Schwartz, C. A. Huber, and A. V. Nurmikko, Proc. Intl. Conf. Narrow-Gap Semiconductors (Linz), 1981.

Supported by the Materials Research Laboratory NSF and the AFOSR.

Summaries of Other Related Work

Microstructure and Fracture Toughness of Cemented Carbides - J. Gurland (Engineering) - cf. Section 2.

Photoelectrolysis - A. Wold (Engineering) - cf. Section 7.

Hydrodesulfurization Catalysts - A. Wold (Engineering) - cf. Section 7.

Semiconductor Powder Processing for Photovoltaic Cells - B. Roessler (Engineering), J. J. Loferski (Engineering), and J. Gurland (Engineering) - cf. Section 7.

Lecturers in the Materials Research Laboratory Program, 1980-81

July 22, 1980

Solid State Discussion Group: Department of Physics, Professor J. Tauc, Brown University, ELECTRONIC RELAXATIONS IN AMORPHOUS SEMI-CONDUCTORS.

July 25, 1980

Solid State Seminar: Department of Physics, Dr. G. Dohler, Max Planck Institute, EXPERIMENTAL AND THEORETICAL STUDIES OF NIPI DOPING SUPERLATTICES.

July 28, 1980

Solid State Seminar: Department of Physics, Professor Manuel Cardona, Max Planck Institute, SOLIDS UNDER PRESSURE, RECENT DEVELOPMENTS.

July 29, 1980

Solid State Seminar: Department of Physics, Professor Manuel Cardona, Max Planck Institute, OPTICAL PROPERTIES OF HYDROGENATED AMORPHOUS SILICON.

July 29, 1980 (August 5, 1980)

Solid State Discussion Group: Department of Physics, Professor J. J. Quinn, Brown University, MEMORY FUNCTION APPROACH TO THE LOCALIZATION PROBLEM.

July 29, 1980

Nuclear Seminar: Department of Physics, Professor A. Askar, Princeton University and Bogazici University, FINITE ELEMENT TECHNIQUES FOR QUANTAL BOUND AND SCATTERING STATES.

August 1, 1980

Solid State Seminar: Department of Physics, Dr. H. Godfrin, C.N.R.S., Grenoble, MULTIPLE EXCHANGE IN SOLID ^3He .

August 5, 1980

Solid State Discussion Group: Department of Physics, Professor Manuel Cardona, Max Planck Institute, HYDROGENATED AMORPHOUS SILICON.

August 7, 1980

Solid State Seminar: Department of Physics, Professor Manuel Cardona, Max Planck Institute, PHONONS IN HEAVILY DOPED SEMICONDUCTORS: ELECTRON-PHONON INTERACTION.

August 12, 1980

Solid State Discussion Group: Department of Physics, Professor J. M. Kosterlitz, University of Birmingham, SPIN GLASSES AND MEAN FIELD THEORY?

August 19, 1980

Solid State Discussion Group: Department of Physics, Professor Manuel Cardona, Max Planck Institute, SYNCHROTON RADIATION AND APPLICATIONS TO SPECTROSCOPY.

August 28, 1980

Solid Mechanics Seminar: Division of Engineering, Professor P. Perzya, Polish Academy of Science, STABILITY PHENOMENA OF DISSIPATIVE SOLIDS WITH INTERNAL DEFECTS AND IMPERFECTIONS.

September 16, 1980

Nuclear Seminar: Department of Physics, Professor W. Glockle, Ruhr-Universitat, APPROACH TOWARDS A RELATIVISTIC THEORY OF INTERACTING PARTICLES.

September 18, 1980

Condensed Matter Seminar: Department of Physics, Professor J. Bonner, University of Rhode Island, SPIN-PEIERLS TRANSITION SYSTEMS.

September 19, 1980

Solid Mechanics Seminar: Division of Engineering, Dr. Haydn Wadley, Harwell Nuclear Establishment, QUANTITATIVE INTERPRETATION OF ACOUSTIC EMISSION DATA FROM DEFORMATION AND FRACTURE.

September 26, 1980

Physics Colloquium: Department of Physics, Professor C. Elbaum, Brown University, AN INTRODUCTION TO DISLOCATIONS.

September 29, 1980

Solid Mechanics Seminar: Division of Engineering, Professor James Rice, Brown University, CREEP CAVITATION OF GRAIN BOUNDARIES.

October 2, 1980

Condensed Matter Seminar: Department of Physics, Dr. S. Kirkpatrick, IBM, Watson Research Center, EDWARDS-ANDERSON ORDERING IN INFINITE-RANGED SPIN GLASSES.

October 6, 1980

Physics Colloquium: Department of Physics, Dr. C. Shank, Bell Laboratories, INVESTIGATION OF NON-EQUILIBRIUM TRANSPORT IN GaAs USING PICOSECOND OPTICAL TECHNIQUES.

October 6, 1980

Condensed Matter Seminar: Department of Physics, Dr. T. Theis, IBM Watson Research Center, GRATING-ENHANCED LIGHT EMISSION FROM TUNNEL JUNCTIONS.

October 9, 1980

Solid State Seminar: Division of Engineering, Dr. Jerzy Najar, University of Notre Dame, ON THE CRITERION OF TRANSITION FROM PLASTICITY TO HYDRODYNAMICS AT HIGH STRAIN RATES.

October 10, 1980

Mathematics and Applied Mathematics, P.D.E. Seminar: Division of Applied Mathematics, Dr. Bernard Dacorogna, Brown University, NON-CONVENTIONAL VARIATIONAL PROBLEM AND THE SHAPE OF CRYSTALS.

October 10, 1980

Physics Colloquium: Department of Physics, Professor W. R. Gentry, University of Minnesota, PULSED MOLECULAR BEAM EXPERIMENTS.

October 14, 1980

Solid Mechanics Seminar: Division of Applied Mathematics and Division of Engineering, Professor Keiiti Aki, M.I.T., PREDICTION OF STRONG MOTION FOR A POTENTIAL EARTHQUAKE FAULT.

October 16, 1980

Condensed Matter Seminar: Department of Physics, Dr. Daniel Fisher, Bell Laboratories, TWO DIMENSIONAL COMMENSURATE-INCOMMENSURATE TRANSITIONS.

October 23, 1980

Chemistry Colloquium: Department of Chemistry, Dr. John Overend, University of Minnesota, INFRARED SPECTROSCOPY OF ABSORBATES IN LOW-AREA SURFACES.

October 23, 1980

Condensed Matter Seminar: Department of Physics, Professor Fred Pollak, Brooklyn College of C.U.N.Y., MODULATION SPECTROSCOPY FOR FUN AND PROFIT.

October 24, 1980

Chemistry Colloquium: Department of Chemistry, Dr. J. Peter Toennies, Max Planck Institute, ROTATIONAL AND VIBRATIONAL EXCITATION OF MOLECULES IN SINGLE COLLISIONS.

October 27, 1980

Mechanics of Solids and Materials Science—Joint Seminar: Brown University Materials Research Laboratory, Dr. N. J. Petch, University of Strathclyde, Scotland, THE PLASTIC DEFORMATION OF POLYCRYSTALLINE ALUMINUM.

October 27, 1980

Physics Colloquium: Department of Physics, Professor N. Geordano, Purdue University, LOCALIZATION IN THIN WIRES.

October 28, 1980

Mechanics of Solids and Materials Science: Division of Engineering, Dr. N. J. Petch, University of Strathclyde, Scotland, THE DUCTILE-BRITTLE CLEAVAGE TRANSITION STEEL.

October 30, 1980

Condensed Matter Seminar: Department of Physics, Dr. Leigh Sneddon, Princeton University, NON-EQUILIBRIUM SYSTEMS: SYMMETRY-BREAKING AND STATISTICAL MECHANICS.

October 31, 1980

Chemistry Colloquium: Department of Chemistry, Dr. M. B. Robin, Bell Laboratories, MULTIPHOTON SPECTROSCOPY AND NONLINEAR PHOTOCHEMISTRY.

November 3, 1980

Solid Mechanics Seminar: Division of Engineering, Professor R. J. Clifton, Brown University, EXPERIMENTS, DISLOCATION DYNAMICS AND THE PRECURSOR DECAY ANOMALY.

November 7, 1980

Chemistry Colloquium: Department of Chemistry, Dr. James Henis, Monsanto Company, COMPOSITE HOLLOW FIBER MEMBRANES FOR GAS SEPARATIONS.

November 10, 1980

Physics Colloquium: Department of Physics, Professor M. Zuckermann, McGill University, PHASE TRANSITIONS AND PHASE SEPARATION IN ARTIFICIAL AND BIOLOGICAL MEMBRANES.

November 13, 1980

Condensed Matter Seminar: Department of Physics, Professor Mark Kastner, M.I.T., DISPERSIVE TRANSPORT IN CHALCOGENIDE GLASSES.

November 14, 1980

Solid Mechanics Seminar: Division of Engineering, Professor A. Paglietti, Università di Cagliari, ON THE ENERGY OF HEAT FLOW AND ITS IMPLICATIONS IN NON-EQUILIBRIUM THERMODYNAMICS.

November 17, 1980

Chemistry Colloquium: Department of Chemistry, Dr. Gideon Fraenkel, Ohio State University, ORGANOLITHIUM COMPOUNDS: CLUSTER STRUCTURE AND EXCHANGE PHENOMENA.

November 17, 1980

Condensed Matter Seminar: Department of Physics, Dr. Malden Nip, University of Chicago, RELATIONS BETWEEN TWO-DIMENSIONED MODELS WITH CONTINUOUSLY VARYING CRITICAL EXPONENTS.

November 17, 1980

Physics Colloquium: Department of Physics, Dr. A. Rahman, Argonne National Laboratory, MOLECULAR DYNAMICS STUDIES OF STRUCTURAL PHASE TRANSITIONS or NEWTON'S LAWS, HIGH SPEED COMPUTERS AND CRYSTALLIZATION.

November 20, 1980

Condensed Matter Seminar: Department of Physics, Dr. H. Madden, Sandia National Laboratory, SURFACE BANDS AND BONDS BY AUGER SPECTROSCOPY.

November 21, 1980

Chemistry Colloquium: Department of Chemistry, Dr. Thomas J. Gray, Olin Corporation, STRONTIUM CONTAINING ELECTRONIC CERAMICS.

November 24, 1980

Physics Colloquium: Department of Physics, Professor P. J. Estrup, Brown University, PHASES ON SOLID SURFACES.

December 1, 1980

Physics Colloquium: Department of Physics, P. Horn, IBM Watson Research Center, If NOISE: INFRARED DIVERGENCES.

December 2, 1980

Chemistry Colloquium: Department of Chemistry, Dr. William Suggs, Bell Laboratories, LIGAND DESIGN AND SYNTHESIS.

December 3, 1980

Nuclear Seminar: Department of Physics, Professor Paul Dean Maycock, George Washington University, PHOTOVOLTAICS: WE CAN MAKE IT HAPPEN.

December 4, 1980

Condensed Matter Seminar: Department of Physics, Professor K. Strauch, Harvard University, NEW HIGH RESOLUTION MAGNETO-OPTICAL STUDIES IN InSb INVOLVING PHONONS AND IMPURITIES.

December 8, 1980

Solid Mechanics Seminar: Division of Engineering, Professor A. Needleman, Brown University, THERMAL BUCKLING OF RAILROAD TRACKS.

December 8, 1980

Physics Colloquium: Department of Physics, Professor K. Strauch, Harvard University, A CRYSTAL-BALL VIEW OF CHARMONIUM.

December 8, 1980

Materials Science Seminar: Division of Engineering, Dr. Serge Hagege, Cornell University and University of Caen, France, STRUCTURE OF GRAIN BOUNDARIES.

December 12, 1980

Chemistry Colloquium: Department of Chemistry, Dr. Noel Cohen, Hoffman-La Roche, TOTAL SYNTHESIS OF OPTICALLY ACTIVE NATURAL PRODUCTS.

December 15, 1980

Solid Mechanics Seminar: Division of Engineering, Professor J. H. Provost, Princeton University, FINITE ELEMENT SOLUTIONS OF ELASTIC/PLASTIC BOUNDARY VALUE PROBLEMS.

December 17, 1980

Materials Science Group—Plasticity of Solids Discussion Group—Joint Seminar: Materials Research Laboratory, Professor M. G. Stevenson, University of New South Wales, PLASTIC DEFORMATION IN MACHINING AND ITS RELATION TO STUDIES OF DYNAMIC PLASTICITY.

December 19, 1980

Condensed Matter Seminar: Department of Physics, Professor John Cardy, U. C. Santa Barbara, DIRECTED PERCOLATION.

January 12, 1981

Solid Mechanics Seminar: Division of Engineering, Dr. J. Klepaczko, Brown University, PROPAGATION TRANSITION TEMPERATURE CRACK DYNAMICS OF STEELS.

January 26, 1981

Solid Mechanics Seminar: Division of Engineering, Professor William D. Stuart, Department of Geological Sciences, EARTHQUAKE FORECAST MODELS.

January 29, 1981

Condensed Matter Seminar: Department of Physics, Dr. Mukamel, IBM-Weizmann Institute, FLUCTUATIONS INDUCED FIRST ORDER TRANSITIONS AND SYMMETRY—BREAKING FIELDS.

January 29, 1981

Theoretical Seminar: Department of Physics, Dr. R. Shankar, Yale University, SOLVABLE MODELS WITH SELF-TRIALLITY IN STATISTICAL MECHANICS AND FIELD THEORY.

February 2, 1981

Physics Colloquium: Department of Physics, Professor N. Ramsey, Harvard University, DIPOLE MOMENTS AND PARITY VIOLATING SPIN ROTATIONS OF THE NEUTRON.

February 5, 1981

Theoretical Seminar: Department of Physics, Dr. N. Andrei, New York University, EXACT SOLUTION OF KONDO PROBLEM.

February 19, 1981

Condensed Matter Seminar: Department of Physics, Dr. C. Varma, Bell Laboratories, ISSUES IN THE INTERACTION OF SUPERCONDUCTIVITY AND LONG RANGE MAGNETIC ORDER.

February 20, 1981

Condensed Matter Seminar: Department of Physics, Professor I. Imry, IBM and Tel Aviv, TRANSPORT IN DISORDERED SYSTEMS AND THE METAL INSULATOR TRANSITION.

February 20, 1981

Solid Mechanics Seminar: Division of Engineering, Dr. Shamita Das, Columbia University, IDEALIZED MODELS OF FAULT BEHAVIOR PRIOR TO DYNAMIC RUPTURE.

February 20, 1981

Chemistry Colloquium: Department of Chemistry, Dr. Barry B. Snider, Princeton University, LEWIS ACID INDUCED CARBON-CARBON BOND FORMING REACTIONS OF ALKENES.

February 23, 1981.

Solid Mechanics Seminar: Division of Engineering, Professor W. Knauss, California Institute of Technology, EXPERIMENTS IN DYNAMIC CRACK PROPAGATION.

February 26, 1981

Theoretical Seminar: Department of Physics, Dr. S. Templeton, MIT, HOW SUPER-RENORMALIZABLE INTERACTIONS CURE THEIR INFRARED DIVERGENCES.

February 27, 1981

Solid Mechanics Seminar: Division of Engineering, Professor H. Kanamori, California Institute of Technology, AN ASPERITY MODEL AND PRECURSORY SEISMICITY PATTERN.

March 2, 1981

Solid Mechanics Seminar: Division of Engineering, Professor J. L. Erickson, The Johns Hopkins University, GIBBS PROBLEMS FOR SOLIDS IN CONTACT WITH FLUIDS.

March 5, 1981

Condensed Matter Seminar: Department of Physics, Professor J. D. Lister, MIT, TANTALIZING PHASE TRANSITIONS IN LIQUID CRYSTALS.

March 5, 1981

Theoretical Seminar: Department of Physics, Professor W. Fischler, University of Pennsylvania, THE THERMODYNAMICS OF THE NON-LINEAR σ MODEL: A TOY FOR HIGH TEMPERATURE QCD.

March 11, 1981

Materials Science Group and Plasticity of Solids Group: Materials Research Laboratory, Dr. J. F. Kocks, Argonne National Laboratory, KINETICS OF NON-UNIFORM DEFORMATIONS.

March 12, 1981

Condensed Matter Seminar: Department of Physics, Dr. Brage Golding, Bell Laboratories, MICROWAVE PHONON AND PHOTON ECHOES FROM COLD GLASSES.

March 13, 1981

Chemistry Colloquium: Department of Chemistry, Dr. Philip D. Magnus, Ohio State University, RECENT DEVELOPMENTS IN THE SYNTHESIS OF NATURAL PRODUCTS.

March 16, 1981

Lefschetz Center for Dynamical Systems Seminar: Division of Applied Mathematics, Professor Carmen Calderer, University of Maryland, RADIAL MOTIONS FOR NONLINEAR ELASTIC AND VISCO-ELASTIC BODIES.

March 17, 1981

Solid Mechanics Seminar: Division of Applied Mathematics and Division of Engineering, Professor Robert Burridge, Courant Institute of Microstructure, POROELASTICITY EQUATIONS DERIVED FROM MICROSTRUCTURE.

March 19, 1981

Applied Mathematics Colloquium: Division of Applied Mathematics, Professor Stuart Altman, University of Maryland, MULTIPARAMETER, NONLINEAR PROBLEMS WITH APPLICATION TO MECHANICS.

March 26, 1981

Condensed Matter Seminar: Department of Physics, Professor James Gorton, Temple University, A REVIEW OF THE THEORY OF SPINODAL DECOMPOSITION.

March 30, 1981

Solid Mechanics Seminar: Division of Engineering, Professor Arnold D. Kerr, University of Delaware, STABILITY OF CONTINUOUSLY SUPPORTED BEAMS AND PLATES.

April 3, 1981

Special Condensed Matter Seminar: Department of Physics, Professor S. C. Moss, University of Houston, STUDIES OF ORDERING IN INTERCALATED GRAPHITE.

April 6, 1981

Seminar in Solid Mechanics: Division of Engineering, Professor Ken Neale, Harvard University, PLASTIC INSTABILITY IN MEMBRANE TUBES.

April 9, 1981

Condensed Matter Seminar: Department of Physics, Professor Alan Heeger, University of Pennsylvania, OF SOLUTIONS AND STORAGE BATTERIES.

April 9, 1981

Applied Mathematics Colloquium: Division of Applied Mathematics, Professor S. Rivlin, Lehigh University, SOME THOUGHTS ON MATERIAL STABILITY.

April 13, 1981

Physics Colloquium: Department of Physics, Professor M. E. Fisher, Cornell University, A PLENTITUDE OF COMMENSURATE PHASES IN A SIMPLE PHYSICAL SYSTEM.

April 16, 1981

Condensed Matter Seminar: Department of Physics, Mr. Jack Rowe, Bell Laboratories, SURFACE ENHANCED RAMAN-SCATTERING IN ULTRA-HIGH VACUUM.

April 22, 1981

Materials Science Seminars: Division of Engineering, Dr. James H. Steele, Jr., Armco Research Center, THE USE OF FRACTOGRAPHIC-MICROSTRUCTURAL CORRELATIONS IN CHARACTERIZING FAILURE MECHANISMS.

April 23, 1981

Condensed Matter Seminar: Department of Physics, Dr. B. Abeles, Corporate Research Laboratories, Exxon, AMORPHOUS HYDROGENATED SILICON: OPTICAL AND TRANSPORT PROPERTIES RELATED TO SOLAR CELLS.

April 27, 1981

Solid Mechanics Seminar: Division of Engineering, Professor T. Wierzbicki, MIT, BOUNDS FOR FINITE DEFLECTIONS DUE TO IMPULSIVE LOADING ON RIGID-PLASTIC STRUCTURES.

April 30, 1981

Condensed Matter Seminar: Department of Physics, Professor R. Pelcovits, Brown University, THE SMECTIC C-A TRANSITION IN BULK LIQUID CRYSTALS.

April 30, 1981

Theoretical Seminar: Department of Physics, Professor C. Sommerfield, Yale University, CONSTRUCTION OF FERMIONS FROM BOSONS IN THREE SPATIAL DIMENSIONS.

May 4, 1981

Solid Mechanics Seminar: Division of Engineering, Professor John M. Ball, Heriot-Watt University, CAVITATION IN NONLINEAR ELASTICITY.

May 8, 1981

Condensed Matter Seminar: Department of Physics, Professor D. E. Aspnes, Bell Laboratories, CLAUDIUS-MOSSOTTI AND BEYOND: THE OPTICAL PROPERTIES OF HETEROGENEOUS MATERIALS.

May 11, 1981

Solid Mechanics Seminar: Division of Engineering, Professor R. James, Brown University, THE MECHANICS OF MARTENSITIC TRANSFORMATIONS.

May 20, 1981

Condensed Matter Seminar: Department of Physics, Dr. Thomas Taylor, Los Angeles Science Laboratory, A LEAD/AUGER/LOSS STUDY OF OXYGEN ADSORPTION $\text{Bi}^{(001)}$.

May 22, 1981

Solid Mechanics Seminar: Division of Engineering, Professor S. Kaliszky, Technical University of Budapest, OPTIMAL DESIGN OF DYNAMICALLY LOADED RIGID-PLASTIC STRUCTURES.

June 17, 1981

Solid Mechanics Seminar: Division of Engineering, Professor R. S. J. Corran, Oxford University, PLATE IMPACT AT ABOUT 200 ms^{-1} .

List of Staff in the Materials Research Laboratory Program

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<i>NAME</i>	<i>TITLE</i>
C. Elbaum	Professor (Physics)
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K. Kim	Assistant Professor (Research)
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J. J. Quinn	Professor
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